



Full wwPDB EM Validation Report ⓘ

May 8, 2023 – 09:59 PM EDT

PDB ID : 8EWI
EMDB ID : EMD-28646
Title : Structure of the human UBR5 HECT-type E3 ubiquitin ligase in a tetrameric form
Authors : Wang, F.; He, Q.; Lin, G.; Li, H.
Deposited on : 2022-10-23
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

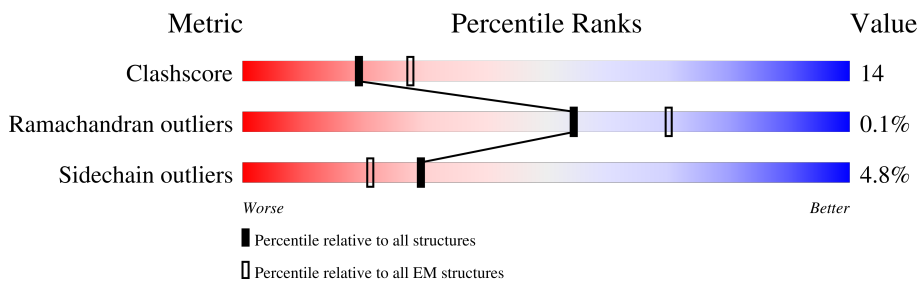
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2799	
1	B	2799	
1	C	2799	
1	D	2799	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 55708 atoms, of which 0 are hydrogens and 0 are deuteriums.

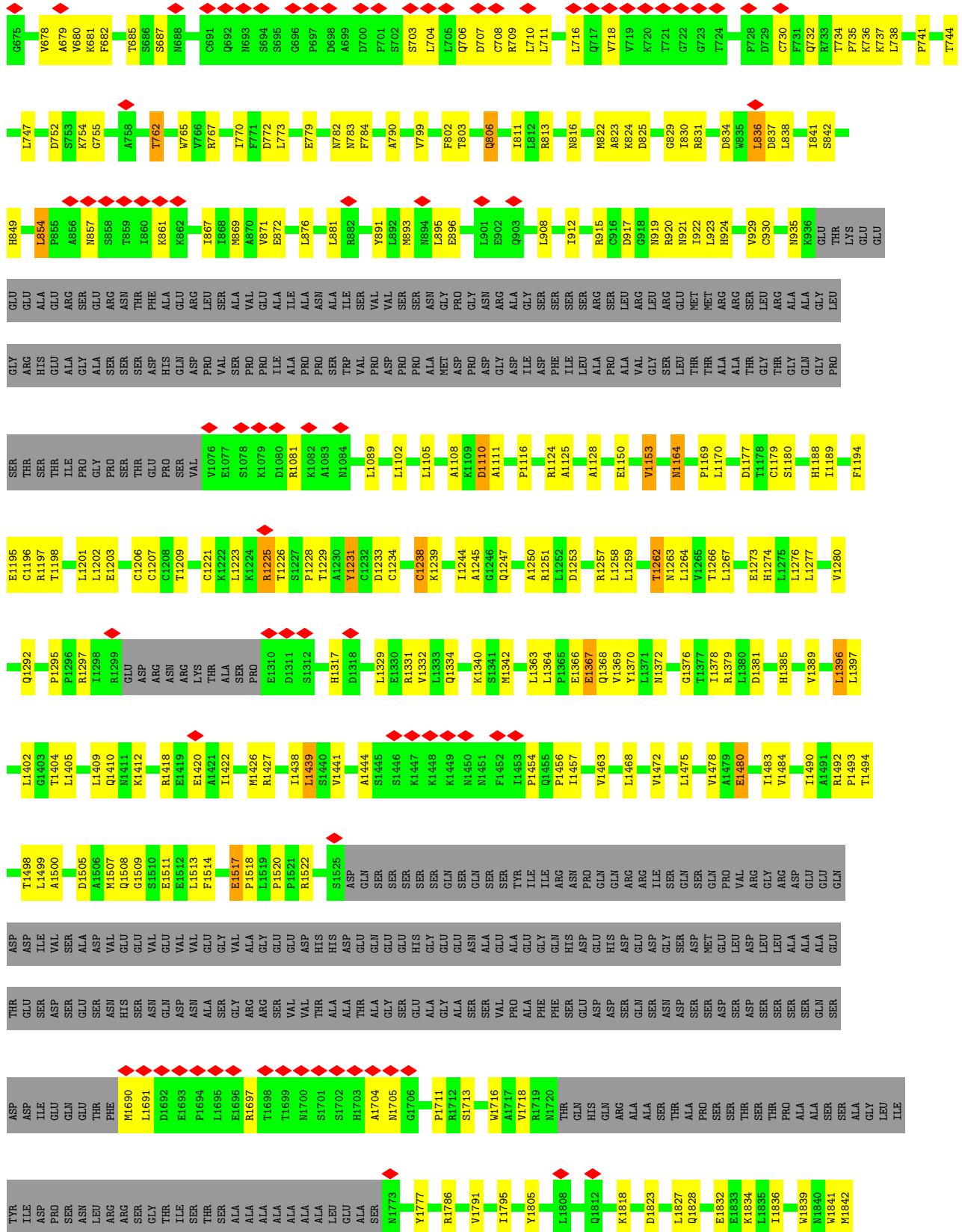
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

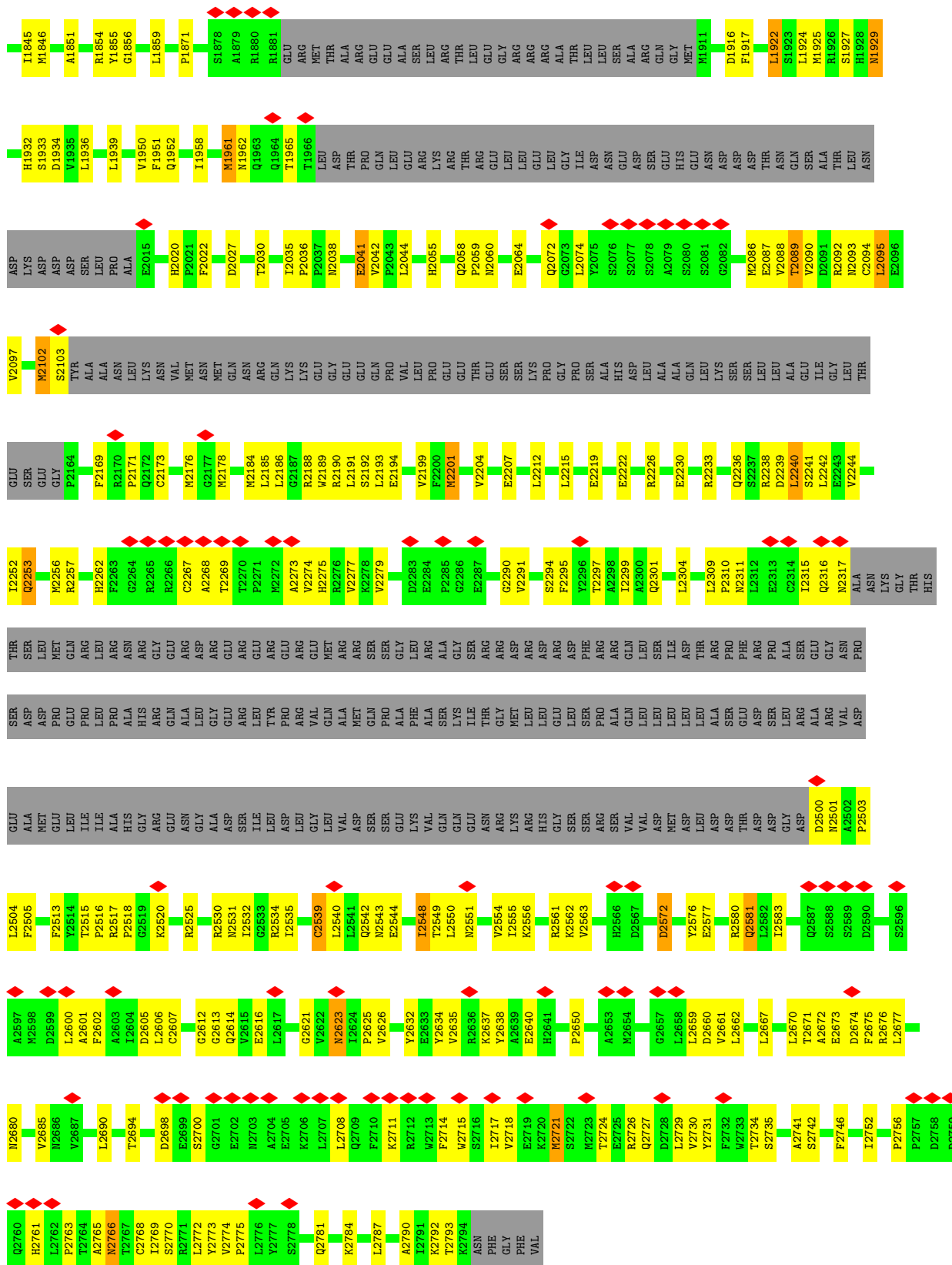
- Molecule 1 is a protein called E3 ubiquitin-protein ligase UBR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1775	13924	8781	2440	2599	104	0	0
1	B	1775	13924	8781	2440	2599	104	0	0
1	C	1775	13924	8781	2440	2599	104	0	0
1	D	1775	13924	8781	2440	2599	104	0	0

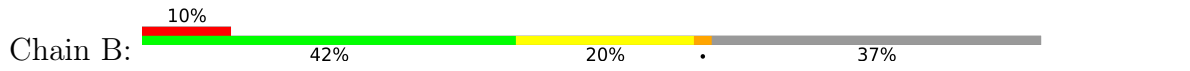
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	3	Total	Zn	0
			3	3	
2	B	3	Total	Zn	0
			3	3	
2	C	3	Total	Zn	0
			3	3	
2	D	3	Total	Zn	0
			3	3	

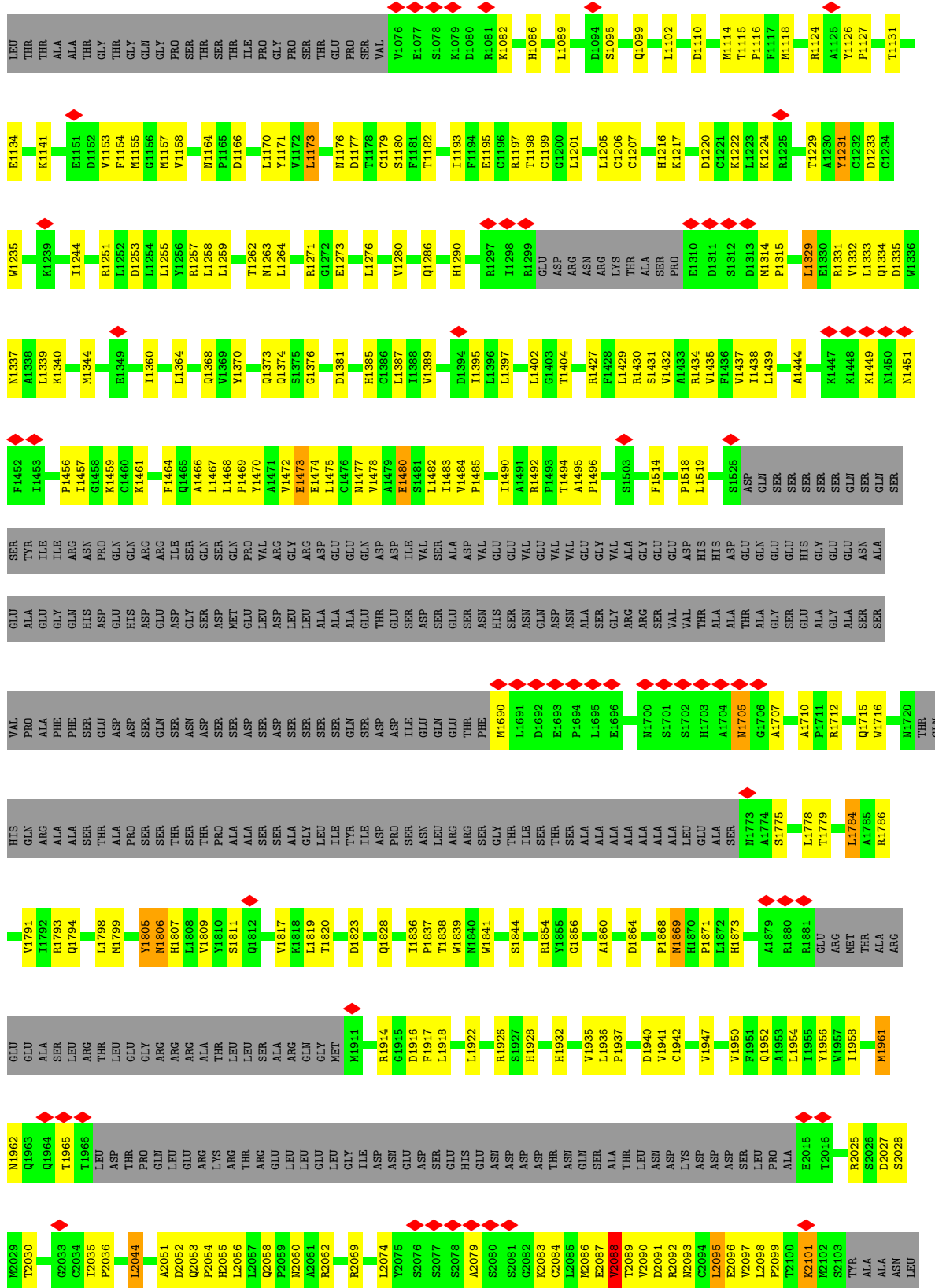


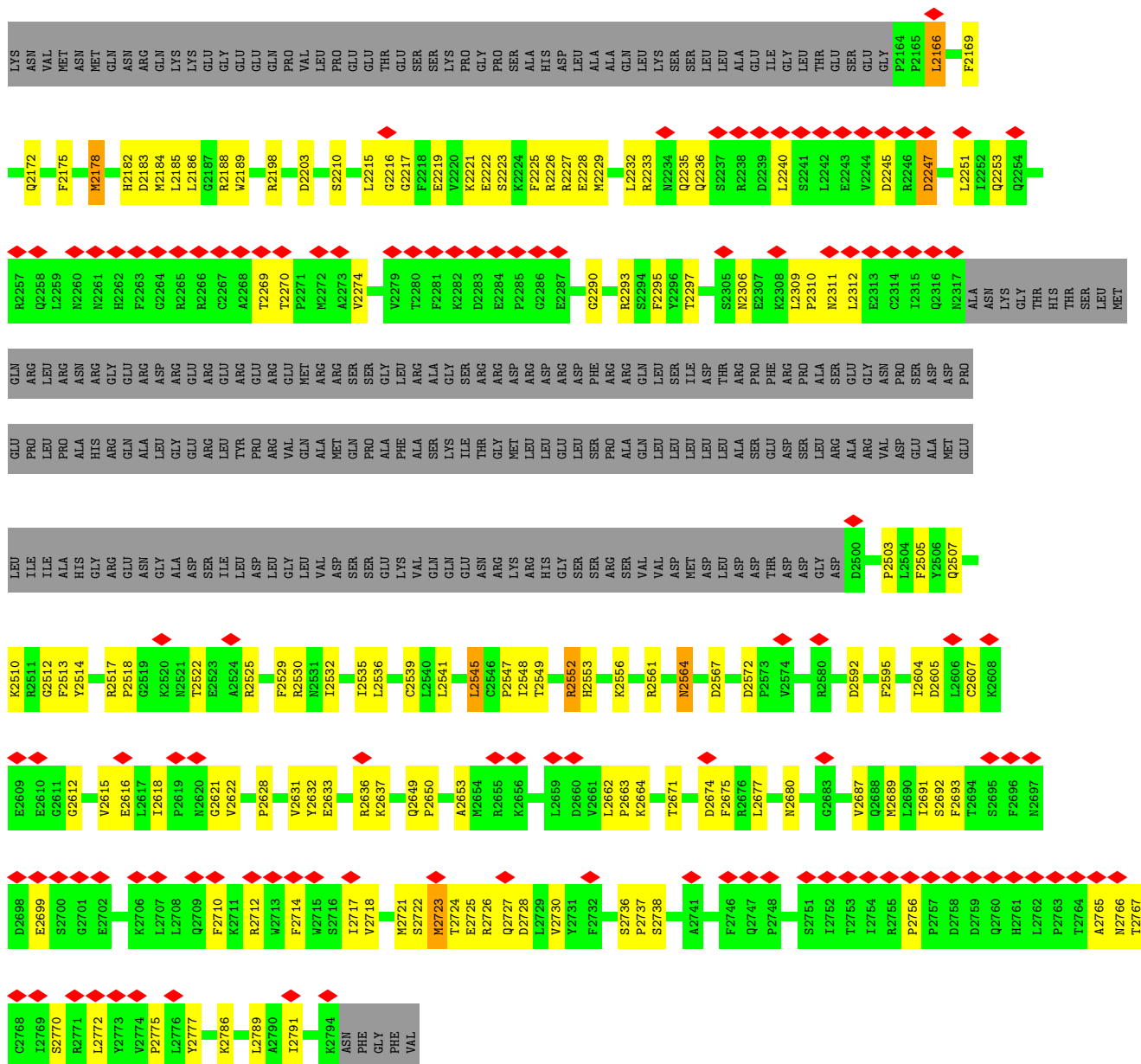


● Molecule 1: E3 ubiquitin-protein ligase UBR5

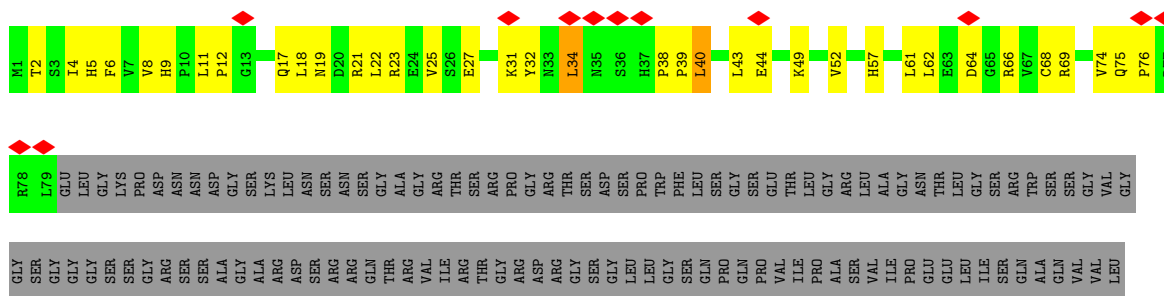
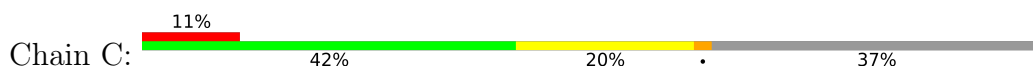


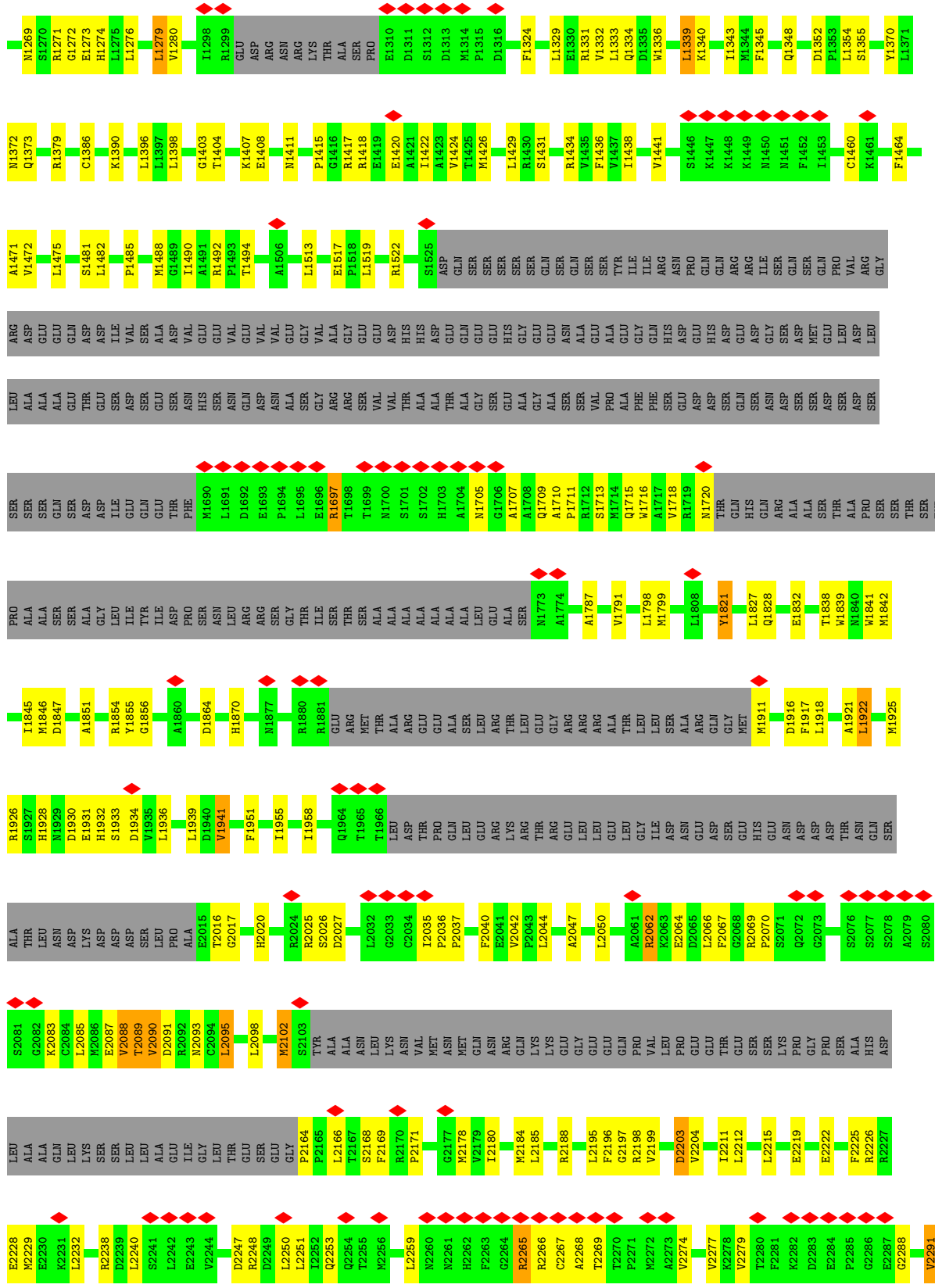
Key amino acid abbreviations and residue numbers visible in the visualization include: H1, T4, H5, H9, P10, L11, P12, E15, D16, Q17, L18, M19, L22, R23, S26, E27, R28, L29, N30, K31, Y32, N33, L34, N35, S36, H37, P38, P39, L40, M41, L43, V44, V52, W53, R69, F72, S73, V74, Q75, P76, D77, R78, L79, and many others down to N919.

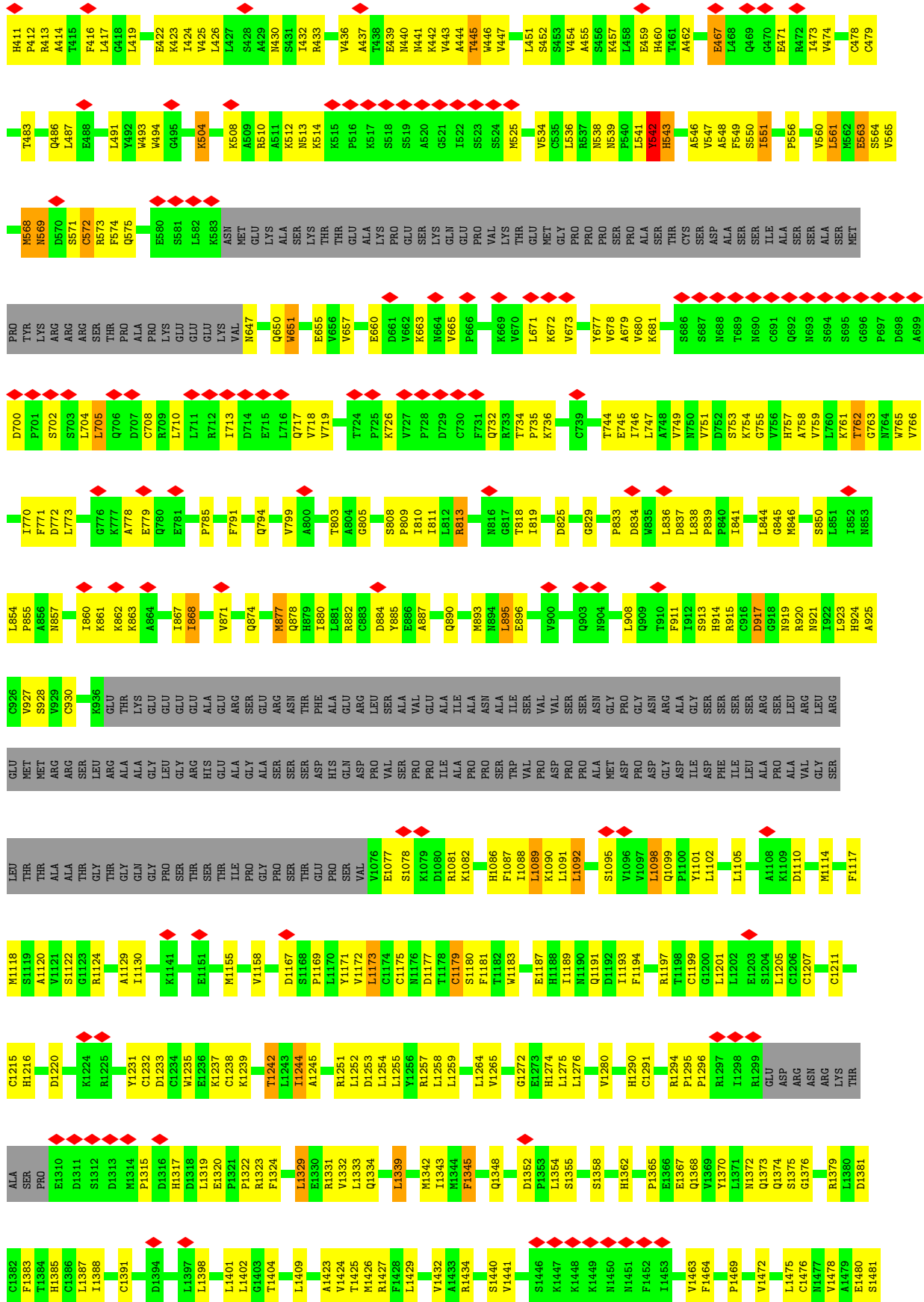


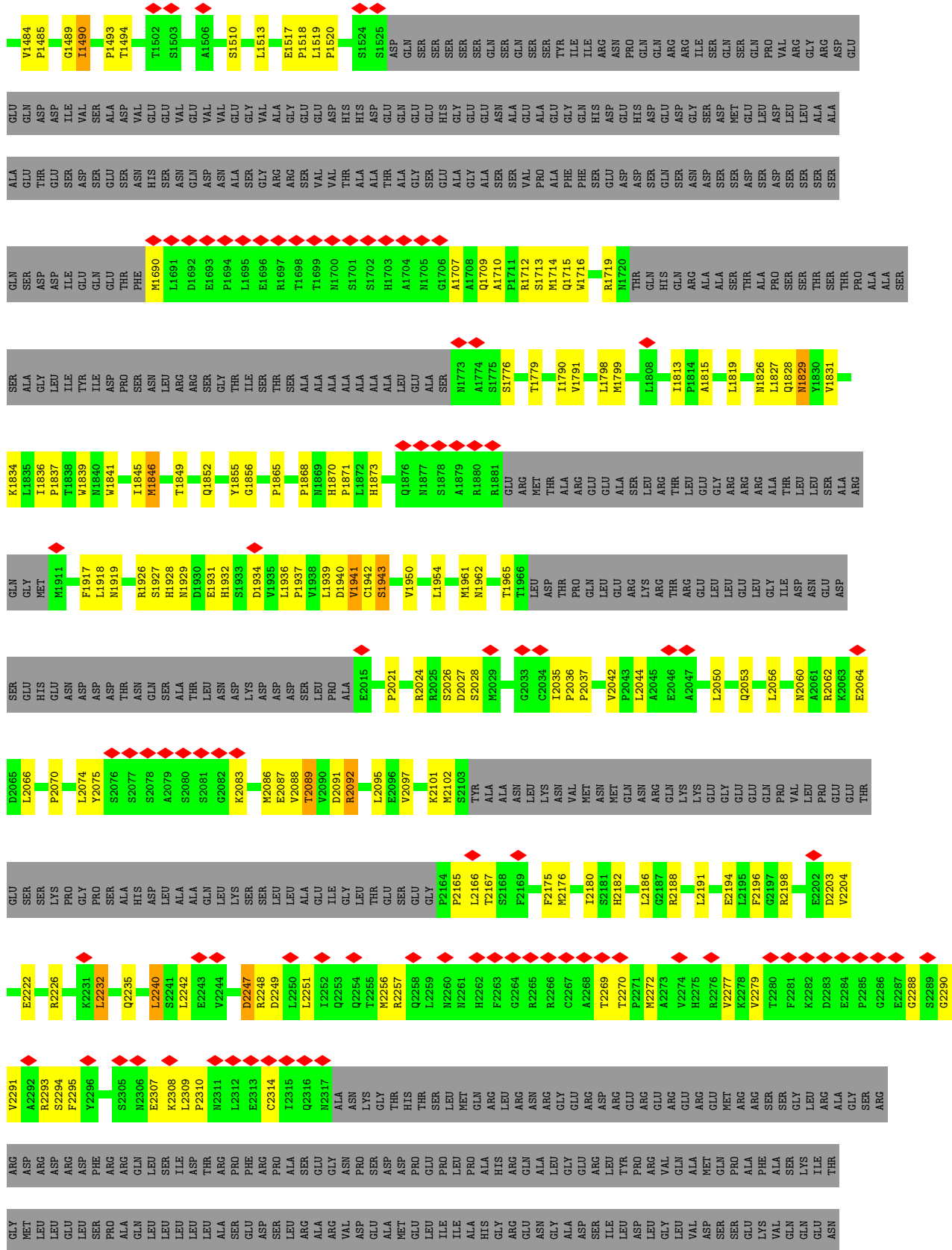


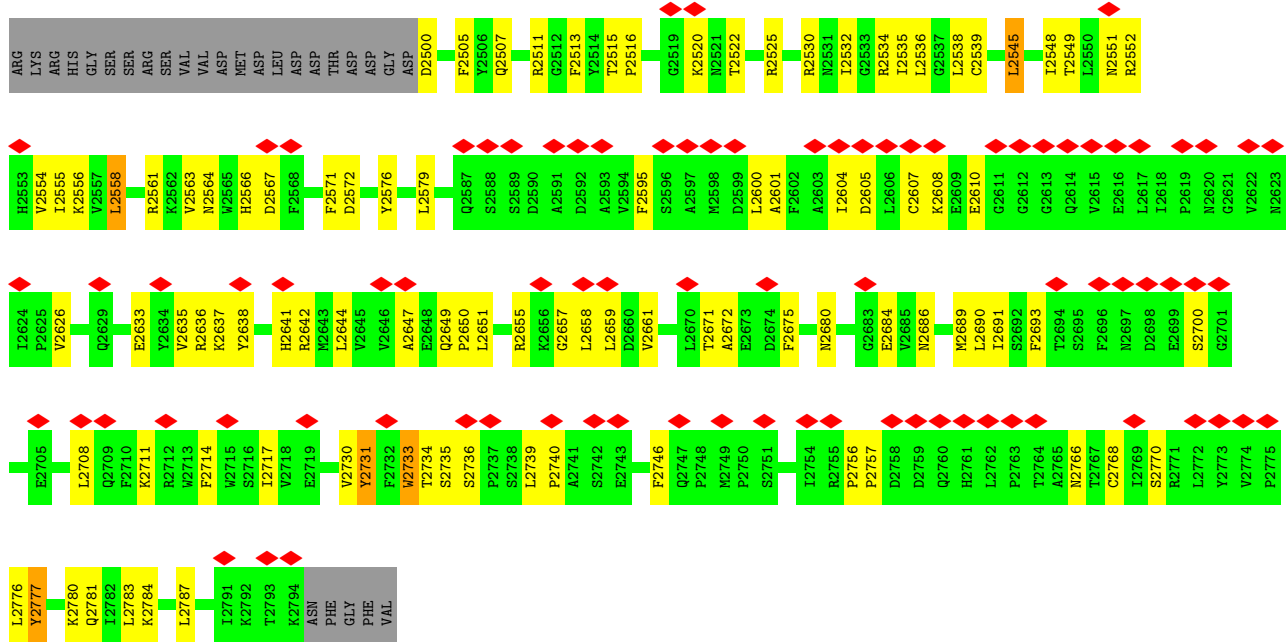
● Molecule 1: E3 ubiquitin-protein ligase UBR5











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	401469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.408	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	364.32, 364.32, 364.32	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/14211	0.48	0/19260
1	B	0.26	0/14211	0.48	0/19260
1	C	0.26	0/14211	0.48	0/19260
1	D	0.26	0/14211	0.48	0/19260
All	All	0.26	0/56844	0.48	0/77040

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13924	0	13931	409	0
1	B	13924	0	13931	407	0
1	C	13924	0	13931	433	0
1	D	13924	0	13931	441	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
All	All	55708	0	55724	1583	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2090:VAL:CG2	1:D:1374:GLN:HE22	1.80	0.95
1:C:744:THR:HA	1:C:761:LYS:O	1.69	0.92
1:B:371:PHE:HA	1:B:385:SER:HA	1.53	0.91
1:C:2090:VAL:HG22	1:D:1374:GLN:HE22	1.37	0.89
1:C:680:VAL:O	1:C:709:ARG:HB2	1.72	0.89
1:B:799:VAL:HA	1:B:813:ARG:O	1.76	0.86
1:A:1295:PRO:HG2	1:A:1297:ARG:HE	1.44	0.83
1:C:1333:LEU:HD13	1:C:1339:LEU:HD21	1.64	0.79
1:D:414:ALA:HB1	1:D:419:LEU:HB2	1.63	0.79
1:B:1199:CYS:SG	1:B:1216:HIS:HE1	2.03	0.79
1:B:531:GLY:HA2	1:B:669:LYS:HG3	1.65	0.78
1:A:1961:MET:HG2	1:A:2173:CYS:HB2	1.66	0.78
1:B:426:LEU:HB2	1:B:437:ALA:HB3	1.65	0.78
1:C:772:ASP:HB2	1:C:779:GLU:HB2	1.65	0.77
1:C:1917:PHE:HE2	1:D:1441:VAL:HG11	1.49	0.77
1:A:1933:SER:HB3	1:B:1376:GLY:HA2	1.67	0.77
1:D:1333:LEU:HD23	1:D:1339:LEU:HD21	1.67	0.77
1:C:426:LEU:HB2	1:C:437:ALA:HB3	1.66	0.76
1:D:671:LEU:HD11	1:D:681:LYS:HG2	1.66	0.76
1:B:18:LEU:HD22	1:B:809:PRO:HB2	1.68	0.76
1:B:498:PRO:HG3	1:B:773:LEU:HB2	1.67	0.75
1:D:2649:GLN:HG2	1:D:2650:PRO:HD3	1.69	0.75
1:D:473:ILE:HG22	1:D:487:LEU:HG	1.69	0.74
1:C:841:ILE:HA	1:C:871:VAL:HA	1.70	0.73
1:C:392:GLN:HE21	1:C:411:HIS:HA	1.52	0.73
1:B:453:SER:O	1:B:457:LYS:NZ	2.22	0.73
1:B:679:ALA:HB1	1:B:708:CYS:HB2	1.69	0.73
1:C:827:MET:HB2	1:C:1197:ARG:HH12	1.53	0.73
1:C:433:ARG:HD3	1:C:478:CYS:HB2	1.70	0.73
1:C:1408:GLU:O	1:C:1418:ARG:NH2	2.22	0.73
1:C:771:PHE:HA	1:C:778:ALA:HA	1.70	0.72
1:B:432:ILE:HG13	1:B:551:ILE:HD12	1.71	0.72
1:B:536:LEU:HB3	1:B:665:VAL:HG11	1.72	0.72
1:D:1177:ASP:H	1:D:1251:ARG:HH22	1.35	0.72
1:C:424:ILE:HG22	1:C:438:THR:HG22	1.71	0.72
1:C:1930:ASP:OD1	1:C:2090:VAL:HG23	1.90	0.71
1:C:62:LEU:HG	1:C:64:ASP:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2102:MET:SD	1:C:2102:MET:N	2.60	0.71
1:A:2661:VAL:HG23	1:A:2662:LEU:HG	1.70	0.71
1:C:1933:SER:HB2	1:D:1376:GLY:HA2	1.71	0.71
1:C:799:VAL:HA	1:C:813:ARG:O	1.90	0.71
1:C:2040:PHE:HB3	1:C:2584:LEU:HD11	1.72	0.71
1:D:744:THR:HG22	1:D:762:THR:HB	1.73	0.71
1:A:2517:ARG:O	1:A:2525:ARG:NH2	2.24	0.71
1:D:1199:CYS:SG	1:D:1216:HIS:HE1	2.10	0.71
1:D:755:GLY:HA2	1:D:773:LEU:HD21	1.73	0.70
1:D:841:ILE:HG12	1:D:871:VAL:HG12	1.72	0.70
1:C:2093:ASN:HB2	1:D:1484:VAL:HG21	1.73	0.70
1:D:917:ASP:OD1	1:D:917:ASP:N	2.23	0.70
1:D:1124:ARG:HH21	1:D:1245:ALA:HA	1.57	0.70
1:D:2028:SER:OG	1:D:2561:ARG:NH2	2.24	0.70
1:D:446:TRP:HB2	1:D:459:GLU:HG3	1.73	0.70
1:A:824:LYS:O	1:A:831:ARG:NH1	2.25	0.70
1:C:1205:LEU:HD13	1:C:1237:LYS:HE3	1.74	0.70
1:D:678:VAL:HG13	1:D:713:ILE:HG12	1.73	0.70
1:B:535:CYS:SG	1:B:536:LEU:N	2.64	0.70
1:D:2293:ARG:HB3	1:D:2736:SER:HB2	1.72	0.70
1:B:1819:LEU:HB3	1:B:2166:LEU:HD11	1.74	0.69
1:A:14:THR:H	1:A:17:GLN:HE22	1.40	0.69
1:A:680:VAL:O	1:A:709:ARG:HB2	1.92	0.69
1:C:554:GLY:HA3	1:C:850:SER:HB3	1.74	0.69
1:D:772:ASP:OD1	1:D:773:LEU:N	2.26	0.69
1:A:929:VAL:O	1:A:1081:ARG:NH1	2.26	0.68
1:C:915:ARG:NH2	1:C:919:ASN:O	2.25	0.68
1:B:750:ASN:ND2	1:B:801:ILE:O	2.26	0.68
1:A:1454:PRO:HB2	1:A:1456:PRO:HD2	1.74	0.68
1:C:424:ILE:HA	1:C:438:THR:HA	1.74	0.68
1:A:1854:ARG:NH1	1:B:1370:TYR:OH	2.26	0.68
1:B:2293:ARG:NH2	1:B:2770:SER:OG	2.26	0.68
1:A:534:VAL:HG12	1:A:718:VAL:HA	1.74	0.68
1:A:2766:ASN:O	1:A:2770:SER:N	2.26	0.68
1:C:670:VAL:HA	1:C:680:VAL:HG22	1.74	0.68
1:D:451:LEU:O	1:D:455:ALA:N	2.23	0.68
1:D:510:ARG:HA	1:D:513:ASN:HB2	1.75	0.68
1:D:2288:GLY:HA3	1:D:2768:CYS:HA	1.75	0.68
1:D:1197:ARG:HB3	1:D:1220:ASP:HB3	1.74	0.68
1:C:2090:VAL:HG21	1:D:1374:GLN:HE22	1.57	0.67
1:D:1238:CYS:SG	1:D:1239:LYS:N	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1697:ARG:HE	1:B:2691:ILE:HD12	1.58	0.67
1:B:1376:GLY:O	1:B:1427:ARG:NH2	2.26	0.67
1:D:568:MET:SD	1:D:568:MET:N	2.66	0.67
1:D:1171:TYR:O	1:D:1175:CYS:HB2	1.95	0.67
1:A:672:LYS:HB3	1:A:679:ALA:HB3	1.76	0.67
1:A:424:ILE:HG13	1:A:438:THR:HG22	1.75	0.67
1:A:2763:PRO:HA	1:A:2773:TYR:O	1.95	0.67
1:A:2092:ARG:HH11	1:B:1490:ILE:HD12	1.59	0.67
1:C:2248:ARG:NH1	1:C:2305:SER:OG	2.27	0.67
1:C:756:VAL:HG13	1:C:771:PHE:HB2	1.77	0.67
1:A:1916:ASP:OD1	1:B:1492:ARG:NH1	2.27	0.66
1:A:433:ARG:NH1	1:A:481:LEU:O	2.28	0.66
1:D:1280:VAL:HG22	1:D:1329:LEU:HD11	1.77	0.66
1:C:759:VAL:HG23	1:C:801:ILE:HD11	1.76	0.66
1:D:538:ASN:O	1:D:542:TYR:N	2.28	0.66
1:D:2766:ASN:O	1:D:2770:SER:HA	1.96	0.66
1:A:710:LEU:HD22	1:C:710:LEU:HD22	1.77	0.66
1:C:2083:LYS:NZ	1:C:2184:MET:SD	2.69	0.66
1:D:1836:ILE:HG13	1:D:1837:PRO:HD3	1.78	0.66
1:B:2290:GLY:HA3	1:B:2767:THR:HB	1.78	0.66
1:C:1494:THR:HG21	1:D:1917:PHE:HB2	1.78	0.66
1:D:447:VAL:HG21	1:D:454:VAL:HG12	1.78	0.66
1:A:562:MET:SD	1:A:563:GLU:N	2.68	0.65
1:B:2044:LEU:HD21	1:B:2051:ALA:HB3	1.77	0.65
1:D:857:ASN:HB3	1:D:862:LYS:HE3	1.78	0.65
1:D:771:PHE:HA	1:D:778:ALA:HA	1.78	0.65
1:D:1839:TRP:NE1	1:D:2176:MET:SD	2.59	0.65
1:B:536:LEU:O	1:B:539:ASN:ND2	2.30	0.65
1:A:2659:LEU:HD21	1:A:2667:LEU:HD22	1.78	0.65
1:B:535:CYS:HB2	1:B:667:VAL:HG22	1.78	0.65
1:A:2685:VAL:HG21	1:A:2730:VAL:HG21	1.79	0.65
1:B:1280:VAL:HG12	1:B:1329:LEU:HD11	1.79	0.65
1:A:1189:ILE:HD12	1:A:1292:GLN:HB3	1.79	0.65
1:B:2186:LEU:HD13	1:B:2215:LEU:HD11	1.78	0.65
1:B:2505:PHE:HB3	1:B:2514:TYR:HB3	1.78	0.65
1:B:1439:LEU:HD21	1:B:1456:PRO:HB2	1.78	0.65
1:B:1712:ARG:HA	1:B:1715:GLN:HG2	1.78	0.65
1:D:11:LEU:HD13	1:D:863:LYS:HE3	1.79	0.65
1:D:799:VAL:HA	1:D:813:ARG:O	1.96	0.65
1:B:1333:LEU:HD23	1:B:1339:LEU:HD21	1.78	0.65
1:C:1847:ASP:OD2	1:C:2188:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:838:LEU:HD12	1:D:839:PRO:HD2	1.77	0.65
1:C:678:VAL:HG21	1:C:716:LEU:HD11	1.77	0.64
1:C:1851:ALA:HB2	1:C:2087:GLU:HB3	1.78	0.64
1:C:2062:ARG:NH1	1:D:1713:SER:OG	2.30	0.64
1:A:854:LEU:HD12	1:A:857:ASN:HA	1.79	0.64
1:D:543:HIS:HB3	1:D:665:VAL:HG11	1.79	0.64
1:D:1826:ASN:O	1:D:1829:ASN:ND2	2.30	0.64
1:C:795:ASN:OD1	1:C:797:ARG:NH1	2.30	0.64
1:B:2549:THR:OG1	1:B:2680:ASN:ND2	2.31	0.64
1:D:401:TYR:CZ	1:D:412:PRO:HD3	2.33	0.64
1:D:1871:PRO:HG3	1:D:1936:LEU:HD11	1.79	0.64
1:B:2222:GLU:OE1	1:B:2226:ARG:NH1	2.31	0.64
1:A:28:LYS:O	1:A:33:ASN:N	2.28	0.64
1:B:2178:MET:SD	1:B:2178:MET:N	2.70	0.64
1:A:394:LYS:HB2	1:A:397:GLU:HG3	1.80	0.64
1:D:2293:ARG:NH2	1:D:2770:SER:OG	2.31	0.64
1:B:69:ARG:HE	1:B:361:GLN:HE21	1.47	0.63
1:D:30:ASN:O	1:D:882:ARG:NH1	2.30	0.63
1:A:72:PHE:HA	1:A:356:LEU:HA	1.80	0.63
1:A:2550:LEU:O	1:A:2676:ARG:NH1	2.26	0.63
1:B:2633:GLU:OE1	1:B:2636:ARG:NH2	2.29	0.63
1:C:2293:ARG:NH2	1:C:2767:THR:O	2.32	0.63
1:D:474:VAL:N	1:D:486:GLN:O	2.30	0.63
1:C:2505:PHE:HB3	1:C:2514:TYR:HB3	1.80	0.63
1:B:363:TRP:HE1	1:B:400:PRO:HB3	1.63	0.63
1:B:2028:SER:OG	1:B:2561:ARG:NH2	2.31	0.63
1:C:1379:ARG:NH1	1:C:1517:GLU:OE1	2.31	0.63
1:B:747:LEU:HD21	1:B:761:LYS:HB2	1.81	0.63
1:B:1334:GLN:HA	1:B:1404:THR:HG21	1.81	0.63
1:D:1155:MET:HA	1:D:1158:VAL:HG12	1.79	0.63
1:C:373:CYS:HB2	1:C:384:VAL:HB	1.81	0.63
1:D:2294:SER:HB3	1:D:2735:SER:HB2	1.81	0.63
1:D:2690:LEU:HG	1:D:2739:LEU:HD21	1.81	0.63
1:C:802:PHE:HB2	1:C:811:ILE:HB	1.80	0.62
1:C:555:ILE:O	1:C:557:LYS:NZ	2.31	0.62
1:D:426:LEU:HG	1:D:437:ALA:HB3	1.82	0.62
1:D:2686:ASN:HD21	1:D:2689:MET:HG3	1.63	0.62
1:D:2766:ASN:ND2	1:D:2768:CYS:SG	2.72	0.62
1:A:1378:ILE:HD11	1:B:1935:VAL:HG23	1.82	0.62
1:B:1166:ASP:HB3	1:B:1217:LYS:HD2	1.81	0.62
1:B:1171:TYR:OH	1:B:1271:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:ASN:ND2	1:C:801:ILE:O	2.32	0.62
1:D:1181:PHE:HB2	1:D:1232:CYS:HB3	1.82	0.62
1:D:1943:SER:OG	1:D:1943:SER:O	2.15	0.62
1:C:6:PHE:HD2	1:C:868:ILE:HD12	1.65	0.62
1:D:1440:SER:HB2	1:D:1790:ILE:HG21	1.81	0.62
1:D:1941:VAL:HG12	1:D:2196:PHE:HE1	1.64	0.62
1:D:2027:ASP:OD1	1:D:2561:ARG:NH2	2.33	0.62
1:A:2240:LEU:HD11	1:A:2277:VAL:HA	1.82	0.62
1:C:748:ALA:HB3	1:C:801:ILE:HG13	1.81	0.62
1:D:473:ILE:HA	1:D:487:LEU:HA	1.82	0.62
1:D:2549:THR:OG1	1:D:2680:ASN:ND2	2.33	0.62
1:A:1438:ILE:HG23	1:B:1918:LEU:HD12	1.81	0.61
1:A:2721:MET:O	1:A:2726:ARG:NH2	2.33	0.61
1:B:2027:ASP:OD1	1:B:2561:ARG:NH2	2.32	0.61
1:B:2724:THR:OG1	1:B:2725:GLU:OE1	2.15	0.61
1:C:2226:ARG:HA	1:C:2229:MET:HG2	1.81	0.61
1:A:2562:LYS:NZ	1:A:2563:VAL:O	2.33	0.61
1:C:1441:VAL:HG11	1:D:1917:PHE:HE2	1.66	0.61
1:A:2637:LYS:HA	1:A:2640:GLU:HB3	1.81	0.61
1:B:818:THR:HA	1:B:840:PRO:HA	1.82	0.61
1:B:2552:ARG:NH1	1:B:2567:ASP:OD1	2.33	0.61
1:A:1367:GLU:OE2	1:B:2069:ARG:NH1	2.34	0.61
1:C:384:VAL:HG23	1:C:427:LEU:HD12	1.81	0.61
1:D:850:SER:HA	1:D:863:LYS:HA	1.83	0.61
1:A:2635:VAL:O	1:A:2638:TYR:HB3	2.01	0.61
1:B:1461:LYS:NZ	1:B:1794:GLN:OE1	2.33	0.61
1:A:62:LEU:HG	1:A:64:ASP:H	1.66	0.61
1:A:1494:THR:HG21	1:B:1917:PHE:HB2	1.83	0.61
1:B:482:TYR:CZ	1:B:773:LEU:HD11	2.36	0.61
1:B:2616:GLU:HG3	1:B:2622:VAL:HG23	1.82	0.61
1:D:1191:GLN:HG3	1:D:1193:ILE:HD11	1.83	0.61
1:D:1385:HIS:NE2	1:D:1510:SER:OG	2.31	0.61
1:A:12:PRO:HD2	1:A:861:LYS:HD3	1.83	0.61
1:B:4:ILE:HG12	1:B:40:LEU:HD22	1.83	0.60
1:A:1331:ARG:NH1	1:A:1331:ARG:O	2.33	0.60
1:D:18:LEU:HD22	1:D:809:PRO:HB2	1.81	0.60
1:A:854:LEU:HD23	1:A:854:LEU:H	1.65	0.60
1:A:1697:ARG:HB3	1:B:2691:ILE:HG23	1.82	0.60
1:C:1718:VAL:HG13	1:D:1942:CYS:HB2	1.83	0.60
1:A:825:ASP:OD1	1:A:829:GLY:N	2.34	0.60
1:C:62:LEU:HD23	1:C:66:ARG:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:ASN:HB3	1:C:803:THR:HG22	1.82	0.60
1:D:414:ALA:HA	1:D:417:LEU:HB2	1.84	0.60
1:A:380:GLU:HB3	1:A:394:LYS:HD3	1.82	0.60
1:A:2240:LEU:HD12	1:A:2241:SER:H	1.66	0.60
1:B:706:GLN:O	1:D:672:LYS:NZ	2.35	0.60
1:C:52:VAL:HG11	1:C:375:GLY:HA2	1.83	0.60
1:A:732:GLN:NE2	1:A:734:THR:O	2.30	0.60
1:A:765:TRP:HE1	1:A:783:ASN:HD22	1.48	0.60
1:B:2087:GLU:O	1:B:2089:THR:N	2.35	0.60
1:C:1713:SER:OG	1:D:2062:ARG:NH1	2.35	0.60
1:A:1124:ARG:NH2	1:A:1177:ASP:O	2.34	0.60
1:A:1258:LEU:HD11	1:A:1264:LEU:HD12	1.82	0.60
1:B:2198:ARG:NH1	1:B:2219:GLU:OE1	2.35	0.60
1:C:795:ASN:ND2	1:C:798:ASN:OD1	2.33	0.60
1:C:544:ALA:HA	1:C:561:LEU:HG	1.83	0.60
1:A:2035:ILE:HD12	1:A:2036:PRO:HD2	1.83	0.60
1:B:744:THR:HG22	1:B:762:THR:HB	1.83	0.60
1:D:1259:LEU:HD11	1:D:1332:VAL:HG22	1.82	0.60
1:C:1928:HIS:HA	1:C:2091:ASP:HB2	1.84	0.60
1:A:930:CYS:HA	1:A:1081:ARG:HH12	1.67	0.59
1:A:1484:VAL:HG21	1:B:2093:ASN:HB2	1.83	0.59
1:A:2721:MET:HG3	1:A:2726:ARG:HH21	1.67	0.59
1:B:814:ASP:OD1	1:B:818:THR:N	2.32	0.59
1:C:2089:THR:HG23	1:D:1373:GLN:HE22	1.65	0.59
1:C:2686:ASN:HB3	1:C:2689:MET:HB2	1.84	0.59
1:D:379:SER:OG	1:D:380:GLU:OE1	2.17	0.59
1:D:1173:LEU:HD12	1:D:1258:LEU:HD22	1.84	0.59
1:D:2522:THR:HG23	1:D:2525:ARG:H	1.67	0.59
1:A:672:LYS:NZ	1:C:708:CYS:O	2.36	0.59
1:A:1929:ASN:OD1	1:B:1430:ARG:NH1	2.35	0.59
1:A:417:LEU:HG	1:A:444:ALA:HB1	1.84	0.59
1:A:2253:GLN:NE2	1:A:2311:ASN:O	2.33	0.59
1:A:672:LYS:HE2	1:A:674:ASP:HB2	1.83	0.59
1:B:475:SER:HB2	1:B:486:GLN:HE21	1.68	0.59
1:D:360:LEU:HD23	1:D:360:LEU:H	1.68	0.59
1:C:678:VAL:HG13	1:C:713:ILE:HG12	1.83	0.59
1:B:771:PHE:HA	1:B:778:ALA:HA	1.84	0.59
1:B:1495:ALA:HA	1:B:1775:SER:H	1.68	0.59
1:D:491:LEU:HD21	1:D:749:VAL:HG11	1.84	0.59
1:C:76:PRO:HG3	1:C:851:LEU:HB3	1.85	0.59
1:C:379:SER:OG	1:C:380:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:785:PRO:HG2	1:D:833:PRO:HD3	1.85	0.59
1:D:2290:GLY:O	1:D:2735:SER:OG	2.20	0.59
1:D:927:VAL:HG21	1:D:1120:ALA:HB2	1.85	0.59
1:B:1793:ARG:HG3	1:B:1956:TYR:HE2	1.68	0.58
1:C:516:PRO:HG2	1:C:717:GLN:HB2	1.84	0.58
1:C:2062:ARG:NH2	1:C:2064:GLU:OE1	2.35	0.58
1:C:1434:ARG:HH21	1:D:1926:ARG:HA	1.67	0.58
1:B:1231:TYR:HD1	1:B:1231:TYR:H	1.50	0.58
1:B:497:VAL:O	1:B:502:ARG:NH1	2.34	0.58
1:C:1485:PRO:HG3	1:D:2092:ARG:HD2	1.85	0.58
1:C:2568:PHE:HZ	1:C:2642:ARG:HD3	1.69	0.58
1:A:1363:LEU:O	1:A:1368:GLN:NE2	2.37	0.58
1:A:1711:PRO:HD3	1:B:2198:ARG:HG2	1.86	0.58
1:B:433:ARG:HH12	1:B:458:LEU:HD13	1.69	0.58
1:B:577:ARG:HD3	1:B:582:LEU:HD21	1.84	0.58
1:B:916:CYS:SG	1:B:917:ASP:N	2.76	0.58
1:C:66:ARG:HB3	1:C:362:TRP:HZ2	1.69	0.58
1:C:2515:THR:HB	1:C:2551:ASN:HD22	1.68	0.58
1:D:2552:ARG:NH1	1:D:2567:ASP:OD1	2.37	0.58
1:A:685:THR:OG1	1:C:672:LYS:NZ	2.37	0.58
1:C:537:ARG:NE	1:C:537:ARG:O	2.35	0.58
1:A:2549:THR:OG1	1:A:2680:ASN:ND2	2.36	0.58
1:B:1331:ARG:O	1:B:1331:ARG:NH1	2.37	0.58
1:C:6:PHE:CD2	1:C:868:ILE:HD12	2.39	0.58
1:C:854:LEU:HD12	1:C:855:PRO:HD2	1.86	0.58
1:C:1930:ASP:OD1	1:C:2090:VAL:CG2	2.51	0.58
1:C:2087:GLU:O	1:C:2089:THR:N	2.36	0.58
1:C:2090:VAL:HG22	1:D:1374:GLN:NE2	2.15	0.58
1:C:2250:LEU:HA	1:C:2253:GLN:HG2	1.85	0.58
1:C:2571:PHE:HE2	1:C:2642:ARG:HB3	1.68	0.58
1:D:673:VAL:HG22	1:D:678:VAL:HG12	1.86	0.58
1:D:2222:GLU:OE1	1:D:2226:ARG:NH1	2.37	0.58
1:B:15:GLU:OE2	1:B:824:LYS:NZ	2.37	0.58
1:B:52:VAL:HB	1:B:376:ALA:HB2	1.86	0.58
1:B:705:LEU:HA	1:D:705:LEU:HB3	1.86	0.58
1:B:850:SER:HA	1:B:863:LYS:HA	1.86	0.58
1:D:560:VAL:O	1:D:574:PHE:HA	2.04	0.58
1:B:432:ILE:HD11	1:B:556:PRO:HG3	1.85	0.57
1:C:551:ILE:HG23	1:C:556:PRO:HB3	1.85	0.57
1:D:75:GLN:HG3	1:D:78:ARG:HB2	1.86	0.57
1:D:1409:LEU:HD11	1:D:1425:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:GLU:HB2	1:A:1277:LEU:HD23	1.86	0.57
1:A:2072:GLN:HB2	1:A:2074:LEU:HD13	1.85	0.57
1:B:2536:LEU:HD11	1:B:2548:ILE:HD11	1.86	0.57
1:C:448:ASP:OD1	1:C:449:GLU:N	2.37	0.57
1:C:2766:ASN:O	1:C:2770:SER:N	2.37	0.57
1:D:1429:LEU:HA	1:D:1432:VAL:HG12	1.86	0.57
1:B:515:LYS:NZ	1:B:517:LYS:O	2.37	0.57
1:B:2306:ASN:HA	1:B:2503:PRO:HB3	1.85	0.57
1:C:1472:VAL:HG21	1:C:1827:LEU:HD21	1.86	0.57
1:A:32:TYR:HB3	1:A:34:LEU:HD23	1.87	0.57
1:B:741:PRO:HG2	1:B:744:THR:HG21	1.86	0.57
1:B:2052:ASP:OD2	1:B:2053:GLN:NE2	2.38	0.57
1:C:18:LEU:HD22	1:C:809:PRO:HB2	1.87	0.57
1:A:1368:GLN:O	1:A:1372:ASN:ND2	2.32	0.57
1:A:2088:VAL:HG13	1:B:1373:GLN:HG3	1.86	0.57
1:A:2503:PRO:O	1:A:2517:ARG:NE	2.28	0.57
1:B:2530:ARG:HE	1:B:2653:ALA:HB1	1.68	0.57
1:D:884:ASP:HB3	1:D:887:ALA:HB3	1.86	0.57
1:A:1179:CYS:SG	1:A:1180:SER:N	2.77	0.57
1:C:2663:PRO:O	1:C:2666:SER:OG	2.20	0.57
1:D:1265:VAL:HG23	1:D:1275:LEU:HD23	1.86	0.57
1:A:360:LEU:HD23	1:A:360:LEU:H	1.70	0.57
1:A:1828:GLN:HE22	1:A:2171:PRO:HB3	1.70	0.57
1:A:1851:ALA:HB2	1:A:2087:GLU:HB3	1.86	0.57
1:B:2216:GLY:O	1:B:2221:LYS:NZ	2.37	0.57
1:C:1918:LEU:HB3	1:D:1513:LEU:HD22	1.85	0.57
1:D:52:VAL:HG11	1:D:375:GLY:HA2	1.87	0.57
1:D:430:ASN:ND2	1:D:478:CYS:O	2.36	0.57
1:D:2062:ARG:NH2	1:D:2064:GLU:OE1	2.38	0.57
1:D:2248:ARG:NH2	1:D:2249:ASP:OD1	2.37	0.57
1:A:1253:ASP:O	1:A:1257:ARG:HG2	2.05	0.57
1:B:924:HIS:CD2	1:B:1116:PRO:HG3	2.40	0.57
1:C:2721:MET:HB3	1:C:2725:GLU:HB2	1.86	0.57
1:B:385:SER:OG	1:B:389:GLU:OE1	2.22	0.57
1:C:682:PHE:O	1:C:685:THR:OG1	2.21	0.57
1:C:2598:MET:HB2	1:C:2600:LEU:HD13	1.87	0.57
1:A:782:ASN:HB3	1:A:830:ILE:HG12	1.87	0.57
1:A:2226:ARG:NH1	1:A:2543:ASN:OD1	2.36	0.57
1:B:929:VAL:O	1:B:1082:LYS:NZ	2.37	0.57
1:D:536:LEU:HG	1:D:538:ASN:H	1.70	0.57
1:D:547:VAL:H	1:D:660:GLU:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:LYS:HB3	1:D:726:LYS:HB2	1.86	0.57
1:A:1238:CYS:SG	1:A:1239:LYS:N	2.77	0.56
1:C:377:LEU:O	1:C:395:TRP:NE1	2.38	0.56
1:C:2259:LEU:HD22	1:C:2534:ARG:HH21	1.70	0.56
1:C:1916:ASP:OD2	1:D:1719:ARG:NH1	2.38	0.56
1:A:1177:ASP:H	1:A:1251:ARG:HH22	1.51	0.56
1:A:2087:GLU:O	1:A:2089:THR:N	2.39	0.56
1:B:479:CYS:SG	1:B:481:LEU:N	2.78	0.56
1:C:2253:GLN:HA	1:C:2312:LEU:HD21	1.86	0.56
1:D:445:THR:HG23	1:D:460:HIS:HB2	1.86	0.56
1:D:1493:PRO:O	1:D:1719:ARG:NH2	2.38	0.56
1:D:1839:TRP:HE3	1:D:1954:LEU:HD13	1.70	0.56
1:B:1271:ARG:NH1	1:B:1273:GLU:OE2	2.38	0.56
1:B:2631:VAL:HG13	1:B:2632:TYR:HD1	1.71	0.56
1:C:473:ILE:HA	1:C:487:LEU:HD13	1.88	0.56
1:A:799:VAL:HA	1:A:813:ARG:O	2.06	0.56
1:A:1925:MET:HB3	1:B:1434:ARG:HG2	1.87	0.56
1:B:893:MET:O	1:B:896:GLU:HG3	2.06	0.56
1:C:2037:PRO:HG3	1:C:2070:PRO:HA	1.87	0.56
1:C:2240:LEU:HD23	1:C:2277:VAL:HG22	1.87	0.56
1:C:2716:SER:OG	1:C:2720:LYS:NZ	2.38	0.56
1:D:2035:ILE:HD12	1:D:2036:PRO:HD2	1.87	0.56
1:A:1124:ARG:HH21	1:A:1245:ALA:HA	1.71	0.56
1:A:2539:CYS:HA	1:A:2544:GLU:HB2	1.87	0.56
1:B:705:LEU:HD22	1:D:704:LEU:HB3	1.88	0.56
1:B:1173:LEU:HD12	1:B:1258:LEU:HD12	1.87	0.56
1:B:2545:LEU:HD13	1:B:2738:SER:HB2	1.86	0.56
1:B:2662:LEU:HD12	1:B:2663:PRO:HD2	1.87	0.56
1:C:568:MET:SD	1:C:568:MET:N	2.79	0.56
1:C:813:ARG:NH1	1:C:842:SER:O	2.37	0.56
1:C:2035:ILE:HD12	1:C:2036:PRO:HD2	1.88	0.56
1:C:2507:GLN:HE22	1:C:2512:GLY:H	1.52	0.56
1:D:1475:LEU:HD22	1:D:1791:VAL:HG23	1.87	0.56
1:A:2561:ARG:NH2	1:A:2670:LEU:O	2.38	0.56
1:B:753:SER:HB3	1:B:806:GLN:HB3	1.88	0.56
1:B:2035:ILE:HD12	1:B:2036:PRO:HD2	1.86	0.56
1:D:1169:PRO:HD2	1:D:1264:LEU:HD11	1.87	0.56
1:A:377:LEU:HD21	1:A:434:ALA:HB2	1.87	0.56
1:C:1709:GLN:O	1:D:2198:ARG:NH2	2.39	0.56
1:C:2274:VAL:H	1:C:2541:LEU:HD21	1.70	0.56
1:C:2517:ARG:NH1	1:C:2518:PRO:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:803:THR:HA	1:D:846:MET:HE2	1.88	0.56
1:B:2240:LEU:HB2	1:B:2274:VAL:HG11	1.87	0.56
1:D:2556:LYS:HE3	1:D:2561:ARG:HE	1.71	0.56
1:A:935:ASN:OD1	1:A:1245:ALA:N	2.38	0.56
1:C:1855:TYR:OH	1:C:1933:SER:O	2.24	0.56
1:C:2198:ARG:NH2	1:C:2219:GLU:OE2	2.39	0.56
1:D:536:LEU:HG	1:D:538:ASN:N	2.20	0.56
1:D:467:GLU:HG3	1:D:735:PRO:HB2	1.88	0.55
1:A:1917:PHE:HB2	1:B:1494:THR:HG21	1.86	0.55
1:A:2038:ASN:HD22	1:A:2041:GLU:H	1.53	0.55
1:A:2252:ILE:HB	1:A:2310:PRO:HG2	1.88	0.55
1:B:757:HIS:ND1	1:B:768:TYR:OH	2.36	0.55
1:C:380:GLU:O	1:C:395:TRP:NE1	2.39	0.55
1:C:565:VAL:HG11	1:C:653:LEU:HD23	1.87	0.55
1:C:2520:LYS:H	1:C:2525:ARG:HH12	1.54	0.55
1:D:1272:GLY:HA3	1:D:1354:LEU:HB2	1.89	0.55
1:B:1253:ASP:O	1:B:1257:ARG:HG2	2.06	0.55
1:C:1265:VAL:O	1:C:1274:HIS:NE2	2.39	0.55
1:A:1329:LEU:HD23	1:A:1397:LEU:HD13	1.88	0.55
1:A:2236:GLN:NE2	1:A:2273:ALA:O	2.39	0.55
1:B:2723:MET:SD	1:B:2723:MET:N	2.78	0.55
1:C:1082:LYS:O	1:C:1086:HIS:ND1	2.36	0.55
1:C:1411:ASN:O	1:C:1418:ARG:NH1	2.39	0.55
1:D:1352:ASP:OD1	1:D:1352:ASP:N	2.39	0.55
1:D:2037:PRO:HG3	1:D:2070:PRO:HA	1.88	0.55
1:D:2500:ASP:HB2	1:D:2520:LYS:HD2	1.88	0.55
1:A:1855:TYR:OH	1:A:1933:SER:O	2.24	0.55
1:B:750:ASN:HB2	1:B:801:ILE:HB	1.89	0.55
1:C:371:PHE:HA	1:C:385:SER:HA	1.88	0.55
1:C:401:TYR:HE1	1:C:403:ASN:HB2	1.72	0.55
1:A:46:ALA:HB1	1:A:62:LEU:HD13	1.89	0.55
1:C:9:HIS:CD2	1:C:865:ALA:HB3	2.42	0.55
1:D:915:ARG:NH1	1:D:921:ASN:OD1	2.40	0.55
1:B:1820:THR:OG1	1:B:1823:ASP:OD1	2.24	0.55
1:B:2054:PRO:HG3	1:B:2510:LYS:HG2	1.89	0.55
1:C:724:THR:HG23	1:C:727:VAL:HG22	1.88	0.55
1:D:1291:CYS:O	1:D:1294:ARG:NH2	2.39	0.55
1:D:2248:ARG:NH2	1:D:2308:LYS:O	2.39	0.55
1:A:704:LEU:HD12	1:C:701:PRO:HB2	1.88	0.55
1:A:2257:ARG:HD3	1:A:2315:ILE:HA	1.89	0.55
1:D:2708:LEU:HD13	1:D:2711:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2244:VAL:HG11	1:A:2295:PHE:HE1	1.72	0.55
1:B:1952:GLN:NE2	1:B:2210:SER:OG	2.38	0.55
1:C:2536:LEU:HD21	1:C:2548:ILE:HD13	1.89	0.55
1:D:413:ARG:HH12	1:D:416:PHE:HB3	1.72	0.55
1:B:542:TYR:O	1:B:565:VAL:N	2.31	0.54
1:B:837:ASP:OD1	1:B:920:ARG:NH2	2.38	0.54
1:C:534:VAL:HG12	1:C:718:VAL:HA	1.88	0.54
1:D:2242:LEU:HD11	1:D:2279:VAL:HA	1.89	0.54
1:D:2734:THR:HG22	1:D:2770:SER:HB3	1.89	0.54
1:B:854:LEU:HD12	1:B:855:PRO:HD2	1.88	0.54
1:B:1468:LEU:O	1:B:1472:VAL:HG22	2.06	0.54
1:C:1934:ASP:HB2	1:D:1518:PRO:HB3	1.88	0.54
1:D:1690:MET:SD	1:D:1690:MET:N	2.80	0.54
1:D:2633:GLU:OE1	1:D:2636:ARG:NH2	2.30	0.54
1:A:19:ASN:ND2	1:A:822:MET:O	2.39	0.54
1:A:43:LEU:HD12	1:A:46:ALA:HB3	1.88	0.54
1:B:441:ASN:O	1:B:464:THR:OG1	2.21	0.54
1:B:1385:HIS:CE1	1:B:1389:VAL:HG11	2.43	0.54
1:C:510:ARG:HB2	1:C:541:LEU:HD11	1.88	0.54
1:C:1911:MET:SD	1:C:1911:MET:N	2.80	0.54
1:A:1170:LEU:HD13	1:A:1258:LEU:HD23	1.89	0.54
1:B:915:ARG:NH2	1:B:919:ASN:O	2.37	0.54
1:C:1352:ASP:OD1	1:C:1352:ASP:N	2.40	0.54
1:D:2637:LYS:O	1:D:2641:HIS:N	2.40	0.54
1:A:708:CYS:O	1:C:672:LYS:NZ	2.33	0.54
1:A:841:ILE:HG22	1:A:871:VAL:HG12	1.89	0.54
1:A:1690:MET:N	1:A:1690:MET:SD	2.81	0.54
1:A:2226:ARG:NE	1:A:2742:SER:OG	2.40	0.54
1:C:1522:ARG:HD3	1:D:1865:PRO:HD3	1.90	0.54
1:A:27:GLU:O	1:A:31:LYS:N	2.34	0.54
1:B:1131:THR:O	1:B:1134:GLU:HG3	2.07	0.54
1:A:1472:VAL:HG21	1:A:1827:LEU:HD21	1.89	0.54
1:C:2180:ILE:HG23	1:C:2185:LEU:HD21	1.90	0.54
1:D:2536:LEU:HD21	1:D:2548:ILE:HB	1.90	0.54
1:A:1711:PRO:HA	1:B:2060:ASN:HD21	1.71	0.54
1:B:411:HIS:CD2	1:B:414:ALA:HB2	2.42	0.54
1:B:1839:TRP:HE3	1:B:1954:LEU:HD13	1.72	0.54
1:B:2098:LEU:HB2	1:B:2099:PRO:HD3	1.90	0.54
1:B:2553:HIS:HB3	1:B:2567:ASP:HB3	1.90	0.54
1:C:838:LEU:N	1:C:917:ASP:OD2	2.37	0.54
1:C:2521:ASN:H	1:C:2525:ARG:HH22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LEU:HG	1:A:908:LEU:HD21	1.90	0.54
1:A:1704:ALA:O	1:A:1705:ASN:ND2	2.41	0.54
1:C:1131:THR:O	1:C:1134:GLU:HG2	2.08	0.54
1:B:747:LEU:HB2	1:B:759:VAL:HG23	1.89	0.54
1:C:817:GLY:HA3	1:C:840:PRO:HB3	1.90	0.54
1:C:837:ASP:N	1:C:917:ASP:OD2	2.41	0.54
1:A:836:LEU:HD13	1:A:838:LEU:HD12	1.90	0.53
1:B:493:TRP:CZ2	1:B:773:LEU:HB3	2.43	0.53
1:B:2309:LEU:HD12	1:B:2310:PRO:HD2	1.90	0.53
1:C:69:ARG:HH22	1:C:395:TRP:HA	1.73	0.53
1:A:2199:VAL:HG22	1:B:1710:ALA:HB2	1.89	0.53
1:C:923:LEU:HD23	1:C:1105:LEU:HB3	1.91	0.53
1:B:572:CYS:SG	1:B:573:ARG:N	2.81	0.53
1:B:1124:ARG:NH1	1:B:1177:ASP:O	2.42	0.53
1:C:27:GLU:O	1:C:31:LYS:N	2.33	0.53
1:C:747:LEU:HD23	1:C:759:VAL:HG12	1.90	0.53
1:C:882:ARG:NH1	1:C:884:ASP:OD2	2.40	0.53
1:C:1821:TYR:OH	1:C:2168:SER:O	2.22	0.53
1:C:2506:TYR:CD1	1:C:2517:ARG:HB2	2.44	0.53
1:A:1396:LEU:HD23	1:A:1396:LEU:H	1.73	0.53
1:B:479:CYS:SG	1:B:806:GLN:NE2	2.68	0.53
1:B:510:ARG:NH2	1:B:539:ASN:H	2.06	0.53
1:C:1839:TRP:HZ3	1:C:1958:ILE:HD11	1.74	0.53
1:D:811:ILE:HG21	1:D:844:LEU:HD21	1.91	0.53
1:D:2515:THR:HG23	1:D:2551:ASN:HD22	1.72	0.53
1:C:760:LEU:HD11	1:C:771:PHE:HZ	1.74	0.53
1:D:1375:SER:HG	1:D:1427:ARG:HH22	1.51	0.53
1:D:1379:ARG:NH2	1:D:1517:GLU:OE1	2.41	0.53
1:C:747:LEU:HB3	1:C:799:VAL:HG21	1.89	0.53
1:D:504:LYS:O	1:D:508:LYS:N	2.41	0.53
1:D:549:PHE:H	1:D:657:VAL:HG12	1.74	0.53
1:D:1320:GLU:HB2	1:D:1323:ARG:HH21	1.73	0.53
1:D:2021:PRO:HA	1:D:2024:ARG:HE	1.74	0.53
1:B:476:LEU:O	1:B:477:HIS:ND1	2.42	0.53
1:B:1195:GLU:OE2	1:B:1224:LYS:NZ	2.36	0.53
1:B:2245:ASP:OD1	1:B:2245:ASP:N	2.42	0.53
1:B:2604:ILE:HD11	1:B:2615:VAL:HB	1.91	0.53
1:C:19:ASN:ND2	1:C:822:MET:O	2.42	0.53
1:D:1197:ARG:NH1	1:D:1220:ASP:OD2	2.41	0.53
1:A:1247:GLN:HG3	1:A:1250:ALA:H	1.72	0.53
1:B:1381:ASP:OD1	1:B:1434:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HG12	1:D:867:ILE:HB	1.90	0.53
1:A:1262:THR:OG1	1:A:1263:ASN:N	2.42	0.53
1:A:2572:ASP:OD1	1:A:2572:ASP:N	2.40	0.53
1:B:1449:LYS:HD2	1:B:1451:ASN:HD21	1.73	0.53
1:C:1492:ARG:NE	1:D:1940:ASP:OD1	2.38	0.53
1:D:1201:LEU:HA	1:D:1205:LEU:HB2	1.90	0.53
1:D:2242:LEU:HD21	1:D:2279:VAL:HG22	1.91	0.53
1:A:411:HIS:HB3	1:A:414:ALA:HB2	1.90	0.52
1:A:1480:GLU:OE1	1:B:1928:HIS:NE2	2.42	0.52
1:A:2505:PHE:HD1	1:A:2516:PRO:HA	1.74	0.52
1:B:75:GLN:NE2	1:B:353:PRO:O	2.42	0.52
1:C:1110:ASP:OD1	1:C:1112:ARG:N	2.33	0.52
1:D:2087:GLU:HG2	1:D:2188:ARG:HH21	1.72	0.52
1:A:1508:GLN:OE1	1:A:1509:GLY:N	2.42	0.52
1:B:2765:ALA:HB2	1:B:2772:LEU:HD23	1.91	0.52
1:C:390:LEU:HD11	1:C:436:VAL:HG21	1.91	0.52
1:C:2564:ASN:N	1:C:2567:ASP:OD2	2.40	0.52
1:A:498:PRO:HG3	1:A:773:LEU:HB2	1.90	0.52
1:B:846:MET:HG3	1:B:867:ILE:HG12	1.91	0.52
1:B:1860:ALA:HB2	1:B:1871:PRO:HG2	1.89	0.52
1:C:1921:ALA:O	1:C:1925:MET:HG3	2.09	0.52
1:A:915:ARG:NH2	1:A:919:ASN:OD1	2.42	0.52
1:A:2734:THR:HG22	1:A:2770:SER:HB2	1.90	0.52
1:B:426:LEU:HD23	1:B:476:LEU:HD12	1.91	0.52
1:D:1082:LYS:O	1:D:1086:HIS:ND1	2.30	0.52
1:D:2731:TYR:O	1:D:2735:SER:HA	2.10	0.52
1:A:1379:ARG:HH12	1:A:1517:GLU:HG3	1.74	0.52
1:B:1690:MET:SD	1:B:1690:MET:N	2.83	0.52
1:B:2517:ARG:O	1:B:2525:ARG:NH2	2.41	0.52
1:C:2537:GLY:HA3	1:C:2661:VAL:HG21	1.91	0.52
1:D:1099:GLN:OE1	1:D:1099:GLN:N	2.42	0.52
1:D:2248:ARG:NH1	1:D:2307:GLU:OE1	2.42	0.52
1:C:49:LYS:O	1:C:49:LYS:NZ	2.33	0.52
1:D:30:ASN:ND2	1:D:837:ASP:O	2.41	0.52
1:D:1215:CYS:SG	1:D:1242:THR:OG1	2.68	0.52
1:A:393:TRP:HB3	1:A:400:PRO:HA	1.91	0.52
1:C:893:MET:O	1:C:896:GLU:HG3	2.10	0.52
1:D:1194:PHE:O	1:D:1207:CYS:N	2.36	0.52
1:A:379:SER:HB2	1:A:450:THR:HG23	1.90	0.52
1:A:2724:THR:O	1:A:2727:GLN:HG3	2.10	0.52
1:B:2025:ARG:HB2	1:B:2030:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:HB	1:C:40:LEU:HD13	1.90	0.52
1:C:363:TRP:CZ2	1:C:391:TYR:HB3	2.45	0.52
1:C:1710:ALA:HA	1:D:2198:ARG:HB3	1.91	0.52
1:C:2259:LEU:HB3	1:C:2534:ARG:HE	1.75	0.52
1:D:753:SER:OG	1:D:754:LYS:NZ	2.38	0.52
1:D:837:ASP:N	1:D:917:ASP:OD2	2.43	0.52
1:D:2780:LYS:O	1:D:2784:LYS:HG2	2.10	0.52
1:A:75:GLN:NE2	1:A:353:PRO:O	2.43	0.52
1:A:655:GLU:N	1:A:655:GLU:OE1	2.43	0.52
1:A:770:ILE:O	1:A:779:GLU:N	2.43	0.52
1:C:75:GLN:OE1	1:C:75:GLN:N	2.43	0.52
1:D:571:SER:HB3	1:D:651:TRP:HE3	1.73	0.52
1:A:41:ASN:O	1:A:44:GLU:HB2	2.10	0.51
1:B:2618:ILE:HG13	1:B:2621:GLY:HA3	1.92	0.51
1:C:2603:ALA:HB1	1:C:2614:GLN:HE21	1.76	0.51
1:D:893:MET:O	1:D:896:GLU:HG3	2.10	0.51
1:A:7:VAL:HG21	1:A:21:ARG:HB3	1.93	0.51
1:A:2086:MET:HG3	1:A:2088:VAL:HG23	1.92	0.51
1:B:2233:ARG:HB3	1:B:2541:LEU:HD11	1.91	0.51
1:C:411:HIS:O	1:C:414:ALA:N	2.35	0.51
1:C:474:VAL:N	1:C:486:GLN:O	2.43	0.51
1:C:1411:ASN:HB3	1:C:1418:ARG:HH12	1.75	0.51
1:D:1253:ASP:OD1	1:D:1257:ARG:NH1	2.37	0.51
1:B:498:PRO:O	1:B:501:GLN:NE2	2.41	0.51
1:B:2522:THR:HG23	1:B:2525:ARG:H	1.76	0.51
1:C:2069:ARG:NH1	1:D:1367:GLU:OE2	2.44	0.51
1:C:2267:CYS:SG	1:C:2268:ALA:N	2.84	0.51
1:D:400:PRO:HG2	1:D:402:ARG:HE	1.75	0.51
1:D:1077:GLU:O	1:D:1081:ARG:N	2.39	0.51
1:B:1799:MET:HE1	1:B:2169:PHE:HE2	1.76	0.51
1:C:515:LYS:HG3	1:C:516:PRO:HD3	1.92	0.51
1:C:2572:ASP:N	1:C:2572:ASP:OD1	2.43	0.51
1:D:433:ARG:HG2	1:D:447:VAL:HG12	1.93	0.51
1:D:390:LEU:HD13	1:D:411:HIS:CD2	2.46	0.51
1:D:1855:TYR:OH	1:D:1934:ASP:N	2.43	0.51
1:D:2089:THR:HB	1:D:2095:LEU:HD11	1.93	0.51
1:A:2199:VAL:HG13	1:B:1707:ALA:HA	1.91	0.51
1:B:575:GLN:NE2	1:B:648:GLU:OE1	2.43	0.51
1:C:74:VAL:H	1:C:849:HIS:HE1	1.56	0.51
1:C:493:TRP:HE1	1:C:736:LYS:HE2	1.76	0.51
1:D:424:ILE:HG23	1:D:436:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2558:LEU:HD22	1:D:2658:LEU:HD13	1.92	0.51
1:A:4:ILE:O	1:A:5:HIS:ND1	2.43	0.51
1:A:1444:ALA:HA	1:A:1499:LEU:HG	1.92	0.51
1:A:2184:MET:HG3	1:A:2185:LEU:HD22	1.91	0.51
1:A:2761:HIS:HB3	1:A:2775:PRO:HG3	1.92	0.51
1:B:27:GLU:HG2	1:B:31:LYS:HD2	1.92	0.51
1:B:1193:ILE:HB	1:B:1206:CYS:HB3	1.93	0.51
1:B:1333:LEU:HA	1:B:1339:LEU:HD21	1.92	0.51
1:B:1496:PRO:HA	1:B:1779:THR:HG21	1.93	0.51
1:C:4:ILE:O	1:C:5:HIS:ND1	2.44	0.51
1:D:1841:TRP:CZ3	1:D:1950:VAL:HG21	2.46	0.51
1:A:837:ASP:OD1	1:A:920:ARG:NH2	2.44	0.51
1:A:1475:LEU:HD22	1:A:1791:VAL:HG23	1.91	0.51
1:B:414:ALA:O	1:B:418:GLY:N	2.44	0.51
1:C:2602:PHE:HD2	1:C:2617:LEU:HB2	1.75	0.51
1:D:2766:ASN:O	1:D:2770:SER:CA	2.59	0.51
1:A:49:LYS:HD3	1:A:63:GLU:HG3	1.93	0.51
1:A:1859:LEU:HG	1:B:1519:LEU:HD23	1.92	0.51
1:A:2605:ASP:HA	1:A:2614:GLN:HA	1.92	0.51
1:B:473:ILE:HA	1:B:487:LEU:HD13	1.93	0.51
1:B:1220:ASP:OD1	1:B:1222:LYS:NZ	2.33	0.51
1:C:433:ARG:NE	1:C:483:THR:OG1	2.39	0.51
1:D:745:GLU:HG2	1:D:746:ILE:H	1.75	0.51
1:D:1290:HIS:HE1	1:D:1322:PRO:HG2	1.76	0.51
1:D:2026:SER:OG	1:D:2556:LYS:NZ	2.39	0.51
1:D:2700:SER:HB3	1:D:2756:PRO:HG3	1.93	0.51
1:A:70:ILE:HD13	1:A:360:LEU:HA	1.93	0.51
1:A:2534:ARG:NH1	1:A:2660:ASP:OD2	2.44	0.51
1:B:549:PHE:HA	1:B:558:VAL:HA	1.93	0.51
1:B:1444:ALA:HA	1:B:1786:ARG:HH22	1.76	0.51
1:C:389:GLU:HB2	1:C:391:TYR:CE2	2.46	0.51
1:C:514:LYS:HA	1:C:537:ARG:HH12	1.75	0.51
1:C:1340:LYS:NZ	1:C:1420:GLU:OE2	2.44	0.51
1:D:1868:PRO:HA	1:D:1873:HIS:CE1	2.45	0.51
1:D:2074:LEU:HD13	1:D:2086:MET:HA	1.92	0.51
1:A:1410:GLN:OE1	1:A:1818:LYS:NZ	2.44	0.50
1:A:1916:ASP:OD2	1:B:1492:ARG:NH2	2.40	0.50
1:B:499:PHE:HB3	1:B:654:ARG:CZ	2.41	0.50
1:B:679:ALA:HA	1:B:709:ARG:O	2.11	0.50
1:C:673:VAL:HG22	1:C:678:VAL:HG12	1.93	0.50
1:D:361:GLN:OE1	1:D:361:GLN:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:CYS:HA	1:D:1082:LYS:HD2	1.93	0.50
1:D:2165:PRO:HB2	1:D:2167:THR:HG22	1.92	0.50
1:A:1276:LEU:O	1:A:1280:VAL:HG23	2.11	0.50
1:A:2279:VAL:HG11	1:A:2295:PHE:HB2	1.94	0.50
1:B:390:LEU:HD13	1:B:411:HIS:CD2	2.47	0.50
1:B:500:SER:OG	1:B:654:ARG:NH2	2.42	0.50
1:C:912:ILE:HG23	1:C:1105:LEU:HD21	1.93	0.50
1:C:1201:LEU:HG	1:C:1237:LYS:HD2	1.93	0.50
1:D:854:LEU:HD12	1:D:855:PRO:HD2	1.92	0.50
1:A:2290:GLY:H	1:A:2768:CYS:HA	1.76	0.50
1:B:533:GLN:OE1	1:B:669:LYS:N	2.44	0.50
1:B:2607:CYS:O	1:B:2612:GLY:N	2.42	0.50
1:C:57:HIS:HD2	1:C:69:ARG:HH21	1.58	0.50
1:C:1106:LEU:HD22	1:C:1132:ILE:HD11	1.93	0.50
1:D:762:THR:HG23	1:D:765:TRP:HB3	1.92	0.50
1:D:1712:ARG:HA	1:D:1715:GLN:HG2	1.93	0.50
1:A:1225:ARG:H	1:A:1225:ARG:HD3	1.77	0.50
1:A:1716:TRP:CZ2	1:B:1856:GLY:HA3	2.45	0.50
1:A:2671:THR:OG1	1:A:2673:GLU:OE2	2.26	0.50
1:B:2235:GLN:NE2	1:B:2236:GLN:OE1	2.44	0.50
1:D:2053:GLN:HB2	1:D:2056:LEU:HG	1.94	0.50
1:A:482:TYR:OH	1:A:755:GLY:O	2.29	0.50
1:B:2097:VAL:HG13	1:B:2101:LYS:HD2	1.92	0.50
1:C:1711:PRO:O	1:C:1715:GLN:HG2	2.11	0.50
1:C:1928:HIS:NE2	1:D:1480:GLU:OE2	2.45	0.50
1:D:2050:LEU:HD22	1:D:2066:LEU:HG	1.93	0.50
1:D:2604:ILE:HG21	1:D:2638:TYR:HE2	1.76	0.50
1:A:487:LEU:HB2	1:A:490:SER:HB2	1.94	0.50
1:B:499:PHE:CD1	1:B:654:ARG:HD2	2.47	0.50
1:C:18:LEU:HD21	1:C:811:ILE:HD11	1.93	0.50
1:D:680:VAL:O	1:D:708:CYS:HA	2.12	0.50
1:D:1276:LEU:O	1:D:1280:VAL:HG23	2.11	0.50
1:A:52:VAL:HG22	1:A:374:ILE:HD12	1.94	0.50
1:A:2238:ARG:NH2	1:A:2262:HIS:O	2.44	0.50
1:A:2607:CYS:O	1:A:2612:GLY:N	2.43	0.50
1:A:2729:LEU:HD13	1:A:2787:LEU:HD21	1.94	0.50
1:C:487:LEU:HB2	1:C:490:SER:HB2	1.93	0.50
1:C:514:LYS:HA	1:C:537:ARG:HH22	1.77	0.50
1:C:1279:LEU:HB3	1:C:1329:LEU:HD13	1.93	0.50
1:A:1164:ASN:OD1	1:A:1164:ASN:N	2.44	0.50
1:B:844:LEU:HD13	1:B:869:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:TRP:O	1:D:736:LYS:HB3	2.12	0.50
1:A:654:ARG:H	1:A:654:ARG:HD3	1.77	0.50
1:A:1197:ARG:HH22	1:A:1202:LEU:HB2	1.76	0.50
1:B:1932:HIS:HD2	1:B:1937:PRO:HG3	1.77	0.50
1:C:1926:ARG:HA	1:D:1434:ARG:HH21	1.76	0.50
1:C:2016:THR:HA	1:C:2020:HIS:CD2	2.46	0.50
1:D:2232:LEU:O	1:D:2235:GLN:NE2	2.44	0.50
1:D:2545:LEU:HD21	1:D:2740:PRO:HA	1.94	0.50
1:A:560:VAL:HG22	1:A:575:GLN:HB2	1.93	0.49
1:A:2193:LEU:HD22	1:A:2215:LEU:HD21	1.92	0.49
1:B:2532:ILE:O	1:B:2535:ILE:HG13	2.11	0.49
1:C:501:GLN:HA	1:C:504:LYS:HE2	1.94	0.49
1:C:1334:GLN:HA	1:C:1404:THR:HG21	1.94	0.49
1:C:2042:VAL:HG23	1:C:2047:ALA:HB2	1.94	0.49
1:C:2184:MET:HG3	1:C:2185:LEU:HD22	1.94	0.49
1:D:17:GLN:O	1:D:21:ARG:HG2	2.12	0.49
1:D:2563:VAL:HG11	1:D:2644:LEU:HD11	1.94	0.49
1:A:445:THR:HB	1:A:494:TRP:HH2	1.76	0.49
1:A:710:LEU:HD21	1:C:679:ALA:HB2	1.93	0.49
1:A:1169:PRO:HD2	1:A:1264:LEU:HD13	1.94	0.49
1:A:1514:PHE:HE1	1:B:1922:LEU:HD21	1.77	0.49
1:A:1841:TRP:O	1:A:1845:ILE:HG12	2.11	0.49
1:B:1082:LYS:O	1:B:1086:HIS:ND1	2.35	0.49
1:B:1095:SER:O	1:B:1099:GLN:NE2	2.45	0.49
1:B:1844:SER:OG	1:B:2096:GLU:OE1	2.23	0.49
1:C:821:PRO:HG3	1:C:836:LEU:HD21	1.94	0.49
1:C:886:GLU:OE1	1:C:889:ARG:NH2	2.45	0.49
1:C:1202:LEU:H	1:C:1205:LEU:HB2	1.77	0.49
1:C:2178:MET:SD	1:C:2178:MET:N	2.81	0.49
1:C:2504:LEU:O	1:C:2517:ARG:N	2.45	0.49
1:A:2055:HIS:O	1:A:2058:GLN:NE2	2.32	0.49
1:A:2518:PRO:HB3	1:A:2650:PRO:HG2	1.95	0.49
1:C:401:TYR:CE1	1:C:403:ASN:HB2	2.47	0.49
1:C:1215:CYS:HB2	1:C:1216:HIS:CD2	2.48	0.49
1:C:1276:LEU:O	1:C:1280:VAL:HG23	2.12	0.49
1:C:2240:LEU:HB2	1:C:2277:VAL:HG13	1.94	0.49
1:A:1202:LEU:HG	1:A:1203:GLU:HG2	1.93	0.49
1:A:1492:ARG:NH1	1:B:1916:ASP:OD1	2.32	0.49
1:C:57:HIS:HB2	1:C:395:TRP:CE3	2.47	0.49
1:B:26:SER:HB3	1:B:838:LEU:HG	1.95	0.49
1:B:536:LEU:HA	1:B:717:GLN:OE1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1922:LEU:HG	1:D:1513:LEU:HD21	1.95	0.49
1:C:2274:VAL:HG23	1:C:2542:GLN:HE22	1.78	0.49
1:D:563:GLU:HG2	1:D:573:ARG:HB2	1.94	0.49
1:D:1194:PHE:N	1:D:1207:CYS:O	2.40	0.49
1:A:672:LYS:HG3	1:C:706:GLN:HA	1.94	0.49
1:A:1412:LYS:HZ1	1:A:1418:ARG:HH21	1.60	0.49
1:B:1464:PHE:HB3	1:B:1798:LEU:HD11	1.95	0.49
1:C:2546:CYS:O	1:C:2680:ASN:HA	2.12	0.49
1:D:534:VAL:HA	1:D:719:VAL:H	1.77	0.49
1:D:2579:LEU:HD12	1:D:2635:VAL:HG13	1.93	0.49
1:A:7:VAL:HG12	1:A:867:ILE:HB	1.95	0.49
1:A:1370:TYR:OH	1:B:1854:ARG:HD2	2.12	0.49
1:C:4:ILE:HG13	1:C:43:LEU:HD23	1.94	0.49
1:C:1705:ASN:HA	1:C:1720:ASN:HD21	1.78	0.49
1:D:1519:LEU:HD12	1:D:1520:PRO:HD2	1.95	0.49
1:A:2267:CYS:SG	1:A:2268:ALA:N	2.85	0.49
1:B:1437:VAL:HG11	1:B:1482:LEU:HD11	1.94	0.49
1:B:2228:GLU:HG3	1:B:2232:LEU:HD23	1.95	0.49
1:C:540:PRO:HG3	1:C:566:TRP:CH2	2.48	0.49
1:C:2247:ASP:OD2	1:C:2250:LEU:N	2.42	0.49
1:D:1201:LEU:HD21	1:D:1237:LYS:HG2	1.95	0.49
1:D:1469:PRO:HG3	1:D:1819:LEU:HD13	1.95	0.49
1:D:2601:ALA:HA	1:D:2626:VAL:H	1.78	0.49
1:A:573:ARG:HG2	1:A:650:GLN:HG2	1.93	0.49
1:A:573:ARG:NH1	1:A:648:GLU:OE2	2.46	0.49
1:B:2517:ARG:HD3	1:B:2518:PRO:HD2	1.95	0.49
1:C:455:ALA:HA	1:C:458:LEU:HB2	1.94	0.49
1:D:1841:TRP:O	1:D:1845:ILE:HG12	2.13	0.49
1:D:2647:ALA:HB1	1:D:2651:LEU:HD23	1.95	0.49
1:A:1364:LEU:HD22	1:B:2069:ARG:HH11	1.77	0.49
1:B:425:VAL:HG13	1:B:426:LEU:HD13	1.95	0.49
1:B:2766:ASN:O	1:B:2770:SER:HA	2.12	0.49
1:C:394:LYS:HB2	1:C:397:GLU:HG3	1.95	0.49
1:D:534:VAL:HG13	1:D:718:VAL:HA	1.94	0.49
1:D:549:PHE:HZ	1:D:551:ILE:HG23	1.76	0.49
1:D:1117:PHE:HZ	1:D:1258:LEU:HD11	1.78	0.49
1:D:1331:ARG:O	1:D:1331:ARG:NH1	2.37	0.49
1:D:1348:GLN:NE2	1:D:1372:ASN:O	2.36	0.49
1:D:1375:SER:OG	1:D:1427:ARG:NH2	2.32	0.49
1:D:70:ILE:HD13	1:D:360:LEU:HA	1.93	0.48
1:D:422:GLU:N	1:D:422:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:THR:OG1	1:D:838:LEU:O	2.28	0.48
1:D:846:MET:HG2	1:D:867:ILE:HG23	1.94	0.48
1:D:1087:PHE:O	1:D:1090:LYS:HG2	2.12	0.48
1:D:1122:SER:HA	1:D:1172:VAL:HG11	1.95	0.48
1:A:2677:LEU:O	1:A:2741:ALA:HB2	2.13	0.48
1:B:663:LYS:HB3	1:B:727:VAL:HG23	1.94	0.48
1:B:1914:ARG:O	1:B:1918:LEU:HD23	2.12	0.48
1:B:2592:ASP:OD1	1:B:2592:ASP:N	2.46	0.48
1:C:17:GLN:O	1:C:21:ARG:HG2	2.14	0.48
1:C:1856:GLY:HA3	1:D:1716:TRP:CZ2	2.48	0.48
1:C:1941:VAL:HG11	1:C:2195:LEU:HG	1.94	0.48
1:C:2733:TRP:CD1	1:C:2734:THR:HG23	2.47	0.48
1:D:1091:LEU:O	1:D:1095:SER:N	2.44	0.48
1:D:1388:ILE:HG12	1:D:1398:LEU:HD11	1.95	0.48
1:A:387:LYS:O	1:A:423:LYS:HA	2.13	0.48
1:A:2304:LEU:HD21	1:A:2548:ILE:HA	1.95	0.48
1:B:510:ARG:HA	1:B:510:ARG:HH11	1.78	0.48
1:C:32:TYR:HB3	1:C:34:LEU:HD23	1.95	0.48
1:C:384:VAL:HG13	1:C:424:ILE:HG13	1.93	0.48
1:C:1396:LEU:HD23	1:C:1396:LEU:H	1.77	0.48
1:D:2309:LEU:HD12	1:D:2310:PRO:HD2	1.95	0.48
1:D:2555:ILE:HA	1:D:2558:LEU:HB2	1.95	0.48
1:A:2240:LEU:HA	1:A:2262:HIS:CE1	2.48	0.48
1:B:534:VAL:HG21	1:B:716:LEU:HD13	1.96	0.48
1:C:529:THR:O	1:C:532:THR:OG1	2.27	0.48
1:C:1870:HIS:HD2	1:D:1519:LEU:HD21	1.78	0.48
1:D:394:LYS:HB2	1:D:397:GLU:OE1	2.14	0.48
1:D:2714:PHE:O	1:D:2717:ILE:HG13	2.13	0.48
1:A:539:ASN:N	1:A:540:PRO:HD3	2.29	0.48
1:A:2102:MET:HG2	1:A:2176:MET:SD	2.53	0.48
1:B:403:ASN:ND2	1:B:406:ASN:O	2.46	0.48
1:B:510:ARG:O	1:B:510:ARG:NH1	2.46	0.48
1:B:2605:ASP:OD1	1:B:2605:ASP:N	2.44	0.48
1:C:1828:GLN:HE22	1:C:2171:PRO:HB3	1.78	0.48
1:C:2083:LYS:O	1:C:2188:ARG:NH1	2.46	0.48
1:D:493:TRP:CZ2	1:D:736:LYS:HD2	2.48	0.48
1:D:874:GLN:HG2	1:D:914:HIS:CE1	2.48	0.48
1:D:1464:PHE:HB3	1:D:1798:LEU:HD11	1.96	0.48
1:D:2607:CYS:SG	1:D:2608:LYS:N	2.87	0.48
1:A:14:THR:N	1:A:17:GLN:HE22	2.09	0.48
1:A:1839:TRP:HZ3	1:A:1958:ILE:HD11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1429:LEU:HA	1:B:1432:VAL:HG12	1.96	0.48
1:B:2297:THR:HA	1:B:2547:PRO:HG2	1.94	0.48
1:B:2529:PHE:CD2	1:B:2650:PRO:HB3	2.49	0.48
1:C:2557:VAL:HG21	1:C:2651:LEU:HD13	1.96	0.48
1:A:1207:CYS:HB3	1:A:1234:CYS:HB2	1.95	0.48
1:A:2606:LEU:N	1:A:2613:GLY:O	2.44	0.48
1:A:2714:PHE:O	1:A:2717:ILE:HG13	2.13	0.48
1:B:732:GLN:NE2	1:B:734:THR:O	2.45	0.48
1:C:18:LEU:O	1:C:22:LEU:HG	2.13	0.48
1:C:1174:CYS:HA	1:C:1324:PHE:HE2	1.79	0.48
1:C:2279:VAL:H	1:C:2291:VAL:HG11	1.77	0.48
1:D:1334:GLN:HA	1:D:1404:THR:HG21	1.95	0.48
1:B:510:ARG:NH2	1:B:537:ARG:O	2.38	0.48
1:B:1395:ILE:HD13	1:B:1459:LYS:HE3	1.96	0.48
1:B:2074:LEU:HD23	1:B:2086:MET:HA	1.95	0.48
1:C:747:LEU:HD12	1:C:799:VAL:HG21	1.94	0.48
1:C:1193:ILE:HG23	1:C:1206:CYS:HB2	1.96	0.48
1:A:2020:HIS:CD2	1:A:2022:PHE:H	2.31	0.48
1:C:1711:PRO:HA	1:D:2060:ASN:HD21	1.78	0.48
1:D:1255:LEU:HD11	1:D:1324:PHE:CE1	2.49	0.48
1:D:1272:GLY:O	1:D:1379:ARG:NH1	2.47	0.48
1:D:1423:ALA:O	1:D:1426:MET:HG2	2.13	0.48
1:A:394:LYS:N	1:A:397:GLU:OE2	2.46	0.48
1:A:2277:VAL:HG23	1:A:2542:GLN:HG3	1.96	0.48
1:B:39:PRO:HG2	1:B:40:LEU:HD12	1.95	0.48
1:C:773:LEU:H	1:C:773:LEU:HD22	1.79	0.48
1:C:1352:ASP:O	1:C:1355:SER:OG	2.27	0.48
1:D:6:PHE:HA	1:D:867:ILE:O	2.14	0.48
1:D:2513:PHE:HD2	1:D:2551:ASN:HA	1.78	0.48
1:A:823:ALA:HB3	1:A:831:ARG:HB3	1.95	0.47
1:A:1856:GLY:HA2	1:A:1936:LEU:HD12	1.96	0.47
1:B:757:HIS:HB3	1:B:768:TYR:HE1	1.79	0.47
1:B:1387:LEU:HD11	1:B:1397:LEU:HB3	1.96	0.47
1:B:1469:PRO:HG3	1:B:1819:LEU:HD13	1.95	0.47
1:B:1475:LEU:HA	1:B:1478:VAL:HG12	1.95	0.47
1:B:2775:PRO:HD2	1:B:2777:TYR:HE1	1.78	0.47
1:C:513:ASN:HD21	1:C:726:LYS:HA	1.79	0.47
1:C:2520:LYS:N	1:C:2525:ARG:HH12	2.10	0.47
1:D:1179:CYS:SG	1:D:1180:SER:N	2.87	0.47
1:A:69:ARG:HD2	1:A:395:TRP:CZ3	2.49	0.47
1:A:491:LEU:HB2	1:A:738:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:VAL:HG13	1:A:680:VAL:HG22	1.95	0.47
1:A:923:LEU:HD23	1:A:1105:LEU:HB3	1.97	0.47
1:A:1713:SER:OG	1:B:2062:ARG:NH1	2.47	0.47
1:A:2531:ASN:HA	1:A:2534:ARG:HG2	1.96	0.47
1:B:17:GLN:OE1	1:B:17:GLN:N	2.40	0.47
1:B:532:THR:O	1:B:670:VAL:HG23	2.14	0.47
1:B:2507:GLN:NE2	1:B:2512:GLY:H	2.12	0.47
1:C:52:VAL:HG22	1:C:374:ILE:HD12	1.95	0.47
1:C:549:PHE:CE2	1:C:657:VAL:HG11	2.49	0.47
1:C:739:CYS:N	1:C:776:GLY:O	2.46	0.47
1:C:818:THR:HG21	1:C:917:ASP:HB3	1.95	0.47
1:C:1114:MET:HB3	1:C:1118:MET:HB2	1.95	0.47
1:C:2733:TRP:HD1	1:C:2734:THR:HG23	1.80	0.47
1:D:4:ILE:HG21	1:D:43:LEU:HD23	1.96	0.47
1:D:895:LEU:HD11	1:D:908:LEU:HD13	1.96	0.47
1:D:1841:TRP:HZ3	1:D:1950:VAL:HG21	1.78	0.47
1:D:1927:SER:O	1:D:2091:ASP:HB3	2.13	0.47
1:A:6:PHE:CZ	1:A:356:LEU:HD11	2.49	0.47
1:A:2309:LEU:HG	1:A:2501:ASN:HA	1.97	0.47
1:B:547:VAL:O	1:B:659:VAL:HG12	2.14	0.47
1:B:717:GLN:OE1	1:B:717:GLN:N	2.47	0.47
1:B:834:ASP:OD1	1:B:834:ASP:N	2.47	0.47
1:B:1467:LEU:HD13	1:B:1817:VAL:HG21	1.96	0.47
1:C:931:PHE:CZ	1:C:1123:GLY:HA3	2.50	0.47
1:C:2718:VAL:HA	1:C:2721:MET:SD	2.54	0.47
1:D:536:LEU:O	1:D:539:ASN:HB2	2.15	0.47
1:D:561:LEU:HD22	1:D:563:GLU:H	1.79	0.47
1:D:2610:GLU:OE1	1:D:2610:GLU:N	2.43	0.47
1:A:75:GLN:OE1	1:A:75:GLN:N	2.47	0.47
1:A:1276:LEU:HD13	1:A:1342:MET:HB2	1.96	0.47
1:A:1498:THR:OG1	1:A:1499:LEU:N	2.47	0.47
1:B:2529:PHE:HD2	1:B:2650:PRO:HB3	1.79	0.47
1:C:551:ILE:HA	1:C:556:PRO:HA	1.96	0.47
1:C:1931:GLU:OE1	1:D:1434:ARG:NH2	2.47	0.47
1:C:2044:LEU:HB2	1:C:2576:TYR:CE2	2.49	0.47
1:C:2529:PHE:HA	1:C:2532:ILE:HG22	1.95	0.47
1:D:2605:ASP:OD1	1:D:2605:ASP:N	2.43	0.47
1:A:2765:ALA:HB2	1:A:2772:LEU:HD23	1.95	0.47
1:B:401:TYR:CZ	1:B:412:PRO:HD3	2.50	0.47
1:B:1828:GLN:HB2	1:B:2169:PHE:HZ	1.80	0.47
1:C:540:PRO:HB3	1:C:564:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2195:LEU:HD22	1:D:1714:MET:HE2	1.97	0.47
1:D:702:SER:HA	1:D:705:LEU:HD21	1.97	0.47
1:A:1177:ASP:HA	1:A:1251:ARG:HH12	1.80	0.47
1:A:2087:GLU:OE2	1:A:2188:ARG:NH1	2.47	0.47
1:A:2623:ASN:OD1	1:A:2623:ASN:N	2.42	0.47
1:A:2698:ASP:OD1	1:A:2698:ASP:N	2.48	0.47
1:B:567:ASN:HB3	1:B:570:ASP:HB3	1.97	0.47
1:B:1286:GLN:HG3	1:B:1290:HIS:CE1	2.50	0.47
1:B:2725:GLU:OE1	1:B:2725:GLU:N	2.43	0.47
1:B:2786:LYS:HD2	1:B:2789:LEU:HD21	1.97	0.47
1:C:667:VAL:HG13	1:C:683:PRO:HD2	1.95	0.47
1:C:768:TYR:HB2	1:C:784:PHE:CZ	2.50	0.47
1:C:1234:CYS:SG	1:C:1240:CYS:HB2	2.54	0.47
1:D:2777:TYR:HB2	1:D:2783:LEU:HD22	1.96	0.47
1:A:762:THR:HG23	1:A:765:TRP:HB3	1.97	0.47
1:A:813:ARG:NH1	1:A:841:ILE:O	2.48	0.47
1:A:2504:LEU:HD13	1:A:2532:ILE:HD11	1.96	0.47
1:A:2530:ARG:O	1:A:2534:ARG:HG2	2.14	0.47
1:B:23:ARG:NH1	1:B:835:TRP:O	2.47	0.47
1:B:571:SER:HA	1:B:653:LEU:HB2	1.97	0.47
1:B:1126:TYR:HB2	1:B:1127:PRO:HD3	1.97	0.47
1:B:2097:VAL:O	1:B:2101:LYS:HB2	2.14	0.47
1:C:1488:MET:HG3	1:D:1841:TRP:CD1	2.50	0.47
1:C:1845:ILE:HD12	1:D:1490:ILE:HD12	1.96	0.47
1:D:1089:LEU:HD23	1:D:1092:LEU:HD23	1.95	0.47
1:A:1839:TRP:CZ3	1:A:1958:ILE:HD11	2.50	0.47
1:C:818:THR:HG22	1:C:819:ILE:H	1.79	0.47
1:C:1097:VAL:HG13	1:C:1098:LEU:HG	1.96	0.47
1:C:1343:ILE:HG21	1:C:1424:VAL:HG13	1.97	0.47
1:A:1952:GLN:HE22	1:A:2207:GLU:HB2	1.79	0.47
1:A:2279:VAL:HB	1:A:2291:VAL:HG22	1.97	0.47
1:A:2766:ASN:HB2	1:A:2769:ILE:HG12	1.96	0.47
1:B:463:GLN:HB3	1:B:465:TYR:HE1	1.78	0.47
1:C:827:MET:HB2	1:C:1197:ARG:NH1	2.27	0.47
1:C:1173:LEU:O	1:C:1251:ARG:NH2	2.37	0.47
1:C:2095:LEU:HD13	1:C:2095:LEU:HA	1.67	0.47
1:A:22:LEU:O	1:A:25:VAL:HG12	2.14	0.47
1:B:372:ILE:N	1:B:384:VAL:O	2.40	0.47
1:B:487:LEU:N	1:B:490:SER:O	2.41	0.47
1:B:2217:GLY:O	1:B:2221:LYS:NZ	2.42	0.47
1:C:4:ILE:HG12	1:C:44:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1201:LEU:HD21	1:C:1234:CYS:HA	1.97	0.47
1:C:1280:VAL:HG22	1:C:1329:LEU:HD21	1.95	0.47
1:D:2044:LEU:HB2	1:D:2576:TYR:CE2	2.50	0.47
1:A:38:PRO:N	1:A:39:PRO:HD2	2.30	0.46
1:A:475:SER:OG	1:A:486:GLN:HB3	2.15	0.46
1:A:1378:ILE:HD12	1:A:1518:PRO:HB3	1.98	0.46
1:A:1832:GLU:O	1:A:1836:ILE:HG12	2.14	0.46
1:A:2178:MET:SD	1:A:2178:MET:N	2.88	0.46
1:A:2671:THR:OG1	1:A:2674:ASP:OD2	2.32	0.46
1:B:2718:VAL:O	1:B:2721:MET:HG2	2.16	0.46
1:C:1171:TYR:OH	1:C:1271:ARG:NH2	2.32	0.46
1:D:805:GLY:O	1:D:808:SER:OG	2.33	0.46
1:D:1376:GLY:O	1:D:1427:ARG:NH1	2.49	0.46
1:D:1402:LEU:HD11	1:D:1463:VAL:HG22	1.96	0.46
1:A:371:PHE:HA	1:A:384:VAL:O	2.16	0.46
1:A:924:HIS:CE1	1:A:1110:ASP:HB3	2.49	0.46
1:B:821:PRO:HD2	1:B:835:TRP:CZ3	2.49	0.46
1:B:1841:TRP:CZ3	1:B:1950:VAL:HG11	2.50	0.46
1:B:2091:ASP:OD1	1:B:2092:ARG:N	2.48	0.46
1:B:2311:ASN:OD1	1:B:2312:LEU:N	2.47	0.46
1:C:12:PRO:HD2	1:C:861:LYS:HD3	1.97	0.46
1:C:1842:MET:SD	1:C:1951:PHE:HA	2.55	0.46
1:D:18:LEU:HD11	1:D:811:ILE:HD11	1.97	0.46
1:D:1317:HIS:O	1:D:1317:HIS:ND1	2.49	0.46
1:D:2044:LEU:HB2	1:D:2576:TYR:HE2	1.80	0.46
1:D:2279:VAL:HG21	1:D:2295:PHE:HB3	1.96	0.46
1:D:2572:ASP:OD1	1:D:2572:ASP:N	2.47	0.46
1:A:397:GLU:OE1	1:A:399:GLU:N	2.24	0.46
1:A:530:VAL:HG13	1:A:673:VAL:HB	1.96	0.46
1:B:1431:SER:HA	1:B:1434:ARG:NH1	2.31	0.46
1:B:1705:ASN:HD22	1:B:1705:ASN:H	1.63	0.46
1:C:411:HIS:O	1:C:413:ARG:N	2.47	0.46
1:D:23:ARG:HB2	1:D:836:LEU:HD22	1.96	0.46
1:D:575:GLN:OE1	1:D:647:ASN:ND2	2.49	0.46
1:D:825:ASP:OD1	1:D:829:GLY:N	2.49	0.46
1:A:482:TYR:OH	1:A:752:ASP:O	2.28	0.46
1:A:2240:LEU:HD21	1:A:2277:VAL:HG22	1.98	0.46
1:C:818:THR:HG23	1:C:839:PRO:O	2.15	0.46
1:C:2222:GLU:OE1	1:C:2226:ARG:NH1	2.48	0.46
1:D:2507:GLN:OE1	1:D:2511:ARG:HA	2.16	0.46
1:A:1385:HIS:CD2	1:A:1514:PHE:HD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:ASN:HB2	1:B:1484:VAL:HG21	1.97	0.46
1:B:2054:PRO:HB2	1:B:2513:PHE:CZ	2.50	0.46
1:C:61:LEU:HD22	1:C:374:ILE:HG23	1.98	0.46
1:C:2197:GLY:HA2	1:C:2212:LEU:HB3	1.98	0.46
1:C:2539:CYS:SG	1:C:2540:LEU:N	2.89	0.46
1:D:76:PRO:HB3	1:D:860:ILE:HD13	1.97	0.46
1:D:536:LEU:HD21	1:D:538:ASN:HB3	1.98	0.46
1:D:1388:ILE:HD11	1:D:1432:VAL:HG23	1.97	0.46
1:A:754:LYS:H	1:A:754:LYS:HD2	1.81	0.46
1:A:1195:GLU:O	1:A:1221:CYS:HA	2.16	0.46
1:A:1929:ASN:O	1:A:1929:ASN:ND2	2.44	0.46
1:B:662:VAL:HA	1:B:726:LYS:HB2	1.96	0.46
1:B:1958:ILE:O	1:B:1961:MET:HG3	2.15	0.46
1:C:509:ALA:HA	1:C:512:LYS:HG2	1.96	0.46
1:C:561:LEU:H	1:C:561:LEU:HD23	1.79	0.46
1:C:2601:ALA:HA	1:C:2625:PRO:HA	1.96	0.46
1:C:2708:LEU:HD13	1:C:2711:LYS:HD2	1.97	0.46
1:D:575:GLN:HA	1:D:647:ASN:ND2	2.31	0.46
1:D:794:GLN:HE22	1:D:913:SER:HB3	1.80	0.46
1:D:2191:LEU:O	1:D:2194:GLU:HG3	2.16	0.46
1:A:36:SER:OG	1:A:44:GLU:OE2	2.22	0.46
1:A:806:GLN:N	1:A:806:GLN:OE1	2.49	0.46
1:A:2299:ILE:HG21	1:A:2535:ILE:HD13	1.97	0.46
1:A:2556:LYS:HG2	1:A:2672:ALA:HB2	1.97	0.46
1:A:2583:ILE:HG23	1:A:2632:TYR:HE1	1.81	0.46
1:B:479:CYS:SG	1:B:480:ALA:N	2.89	0.46
1:B:861:LYS:H	1:B:861:LYS:HD2	1.81	0.46
1:B:1429:LEU:HB2	1:B:1474:GLU:HG3	1.98	0.46
1:D:413:ARG:HE	1:D:459:GLU:HG2	1.81	0.46
1:D:1472:VAL:HG21	1:D:1827:LEU:HD21	1.97	0.46
1:A:5:HIS:O	1:A:869:MET:HG2	2.16	0.46
1:A:673:VAL:HG22	1:A:678:VAL:HG12	1.98	0.46
1:A:741:PRO:HB2	1:A:744:THR:HG21	1.98	0.46
1:A:1468:LEU:HD13	1:A:1805:TYR:HE2	1.79	0.46
1:D:1130:ILE:HG12	1:D:1254:LEU:HD13	1.97	0.46
1:D:2203:ASP:OD1	1:D:2204:VAL:N	2.48	0.46
1:A:540:PRO:HD2	1:A:566:TRP:CH2	2.50	0.46
1:A:2027:ASP:HA	1:A:2030:THR:HG22	1.98	0.46
1:B:1869:ASN:OD1	1:B:1869:ASN:N	2.48	0.46
1:A:1381:ASP:OD2	1:B:1926:ARG:NH2	2.47	0.46
1:A:2060:ASN:OD1	1:A:2060:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PRO:HB3	1:B:861:LYS:HG2	1.97	0.46
1:B:770:ILE:O	1:B:779:GLU:N	2.49	0.46
1:C:17:GLN:OE1	1:C:17:GLN:N	2.41	0.46
1:C:1109:LYS:HB3	1:C:1114:MET:N	2.31	0.46
1:D:1828:GLN:O	1:D:1831:VAL:HG12	2.15	0.46
1:D:2564:ASN:HD21	1:D:2566:HIS:HB2	1.80	0.46
1:D:2780:LYS:HE2	1:D:2781:GLN:HE22	1.81	0.46
1:A:790:ALA:HB3	1:A:1111:ALA:HA	1.99	0.45
1:A:1188:HIS:HB3	1:A:1229:THR:OG1	2.16	0.45
1:A:1422:ILE:O	1:A:1426:MET:HG2	2.16	0.45
1:A:2561:ARG:HG2	1:A:2562:LYS:H	1.81	0.45
1:B:1177:ASP:H	1:B:1251:ARG:NH2	2.14	0.45
1:B:1262:THR:OG1	1:B:1263:ASN:N	2.49	0.45
1:B:2723:MET:HA	1:B:2726:ARG:HD2	1.98	0.45
1:C:413:ARG:HH11	1:C:449:GLU:HA	1.81	0.45
1:C:912:ILE:HG13	1:C:1101:TYR:CD1	2.52	0.45
1:C:1098:LEU:HA	1:C:1101:TYR:CD2	2.51	0.45
1:C:1864:ASP:HB3	1:D:1520:PRO:HG2	1.97	0.45
1:C:2507:GLN:NE2	1:C:2512:GLY:H	2.13	0.45
1:C:2698:ASP:OD1	1:C:2698:ASP:N	2.46	0.45
1:D:77:ASP:OD1	1:D:77:ASP:N	2.46	0.45
1:D:766:VAL:HG11	1:D:791:PHE:CD2	2.51	0.45
1:A:1718:VAL:HG13	1:B:1942:CYS:HB3	1.98	0.45
1:B:1947:VAL:HA	1:B:1950:VAL:HG12	1.98	0.45
1:B:1962:ASN:O	1:B:1965:THR:OG1	2.25	0.45
1:B:2699:GLU:HG3	1:B:2756:PRO:HD3	1.97	0.45
1:C:38:PRO:N	1:C:39:PRO:HD2	2.30	0.45
1:C:841:ILE:HG22	1:C:871:VAL:HG12	1.98	0.45
1:D:705:LEU:HD23	1:D:705:LEU:H	1.81	0.45
1:A:502:ARG:NH1	1:A:730:CYS:O	2.50	0.45
1:A:2095:LEU:HD13	1:A:2095:LEU:HA	1.76	0.45
1:B:74:VAL:HG12	1:B:849:HIS:CD2	2.51	0.45
1:B:414:ALA:HA	1:B:417:LEU:HB2	1.99	0.45
1:B:1807:HIS:O	1:B:1811:SER:OG	2.27	0.45
1:C:2644:LEU:O	1:C:2648:GLU:N	2.50	0.45
1:D:423:LYS:HB3	1:D:439:GLU:HB3	1.99	0.45
1:A:445:THR:O	1:A:459:GLU:HG2	2.17	0.45
1:A:1493:PRO:HD2	1:B:1940:ASP:OD2	2.16	0.45
1:B:72:PHE:HE2	1:B:866:VAL:HG21	1.81	0.45
1:B:761:LYS:HA	1:B:765:TRP:O	2.16	0.45
1:B:2689:MET:O	1:B:2692:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:GLU:HB3	1:D:573:ARG:HD3	1.98	0.45
1:D:1235:TRP:CD2	1:D:1315:PRO:HD3	2.52	0.45
1:D:1339:LEU:HD22	1:D:1339:LEU:HA	1.76	0.45
1:D:2279:VAL:HB	1:D:2291:VAL:HG22	1.97	0.45
1:A:816:ASN:HD21	1:A:915:ARG:HG3	1.82	0.45
1:A:834:ASP:OD2	1:A:1239:LYS:NZ	2.49	0.45
1:A:1499:LEU:HD21	1:A:1786:ARG:HH22	1.82	0.45
1:C:738:LEU:HD13	1:C:756:VAL:HG11	1.98	0.45
1:C:1711:PRO:HD3	1:D:2198:ARG:HG3	1.99	0.45
1:C:2531:ASN:O	1:C:2534:ARG:HG2	2.16	0.45
1:D:548:ALA:HB1	1:D:657:VAL:H	1.82	0.45
1:D:1333:LEU:HD22	1:D:1401:LEU:HD13	1.97	0.45
1:D:2534:ARG:HG2	1:D:2661:VAL:HG11	1.97	0.45
1:A:494:TRP:HB3	1:A:735:PRO:HA	1.99	0.45
1:B:40:LEU:HD23	1:B:43:LEU:HD23	1.99	0.45
1:B:2687:VAL:O	1:B:2691:ILE:HG12	2.16	0.45
1:C:1841:TRP:O	1:C:1845:ILE:HG12	2.16	0.45
1:D:549:PHE:CZ	1:D:551:ILE:HG23	2.50	0.45
1:D:1244:ILE:HD13	1:D:1244:ILE:HA	1.77	0.45
1:A:1438:ILE:HD12	1:B:1918:LEU:HD13	1.99	0.45
1:B:460:HIS:ND1	1:B:465:TYR:OH	2.50	0.45
1:B:535:CYS:SG	1:B:665:VAL:HB	2.56	0.45
1:B:1335:ASP:OD1	1:B:1337:ASN:N	2.49	0.45
1:C:495:GLY:O	1:C:732:GLN:HB3	2.16	0.45
1:C:929:VAL:HG23	1:C:1085:ALA:HB1	1.98	0.45
1:C:1237:LYS:HE2	1:C:1237:LYS:HB2	1.81	0.45
1:C:2247:ASP:OD1	1:C:2251:LEU:N	2.49	0.45
1:D:834:ASP:OD1	1:D:834:ASP:N	2.40	0.45
1:A:802:PHE:HB2	1:A:811:ILE:HB	1.99	0.45
1:A:935:ASN:ND2	1:A:1244:ILE:HA	2.31	0.45
1:B:1360:ILE:HD12	1:B:1368:GLN:HA	1.99	0.45
1:B:1839:TRP:CE3	1:B:1954:LEU:HD13	2.51	0.45
1:C:540:PRO:HG2	1:C:543:HIS:NE2	2.32	0.45
1:C:1370:TYR:CD1	1:D:2088:VAL:HG12	2.52	0.45
1:C:1519:LEU:HD21	1:D:1870:HIS:HD2	1.81	0.45
1:C:2740:PRO:HB3	1:C:2745:GLY:HA3	1.99	0.45
1:D:393:TRP:HB3	1:D:400:PRO:HA	1.98	0.45
1:D:510:ARG:HA	1:D:514:LYS:H	1.82	0.45
1:D:671:LEU:HB2	1:D:679:ALA:O	2.17	0.45
1:D:2086:MET:HG3	1:D:2088:VAL:HG22	1.99	0.45
1:D:2757:PRO:HB3	1:D:2776:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:VAL:HG21	1:A:577:ARG:HE	1.82	0.45
1:A:924:HIS:CD2	1:A:1116:PRO:HG3	2.52	0.45
1:A:2219:GLU:O	1:A:2222:GLU:HG3	2.16	0.45
1:B:546:ALA:HB3	1:B:561:LEU:HB3	1.98	0.45
1:B:1793:ARG:HG3	1:B:1956:TYR:CE2	2.51	0.45
1:B:1806:ASN:OD1	1:B:1806:ASN:N	2.49	0.45
1:C:1429:LEU:HD13	1:C:1471:ALA:HA	1.99	0.45
1:A:772:ASP:HB2	1:A:779:GLU:HB2	1.99	0.45
1:B:673:VAL:HG22	1:B:678:VAL:HG12	1.99	0.45
1:B:1154:PHE:HA	1:B:1157:MET:HE2	1.99	0.45
1:B:1402:LEU:HD22	1:B:1467:LEU:HD23	1.98	0.45
1:B:2083:LYS:O	1:B:2188:ARG:NH1	2.50	0.45
1:C:2025:ARG:NH1	1:C:2067:PHE:O	2.48	0.45
1:D:542:TYR:HE2	1:D:546:ALA:H	1.64	0.45
1:D:1098:LEU:HA	1:D:1101:TYR:HD2	1.81	0.45
1:A:424:ILE:HA	1:A:438:THR:HA	1.99	0.44
1:A:935:ASN:HD21	1:A:1244:ILE:HA	1.83	0.44
1:A:1507:MET:O	1:A:1511:GLU:HG2	2.16	0.44
1:A:2500:ASP:HB2	1:A:2520:LYS:HD2	1.97	0.44
1:B:22:LEU:HB3	1:B:836:LEU:HD13	1.97	0.44
1:C:2:THR:OG1	1:C:871:VAL:O	2.24	0.44
1:C:2504:LEU:HB3	1:C:2529:PHE:HE1	1.82	0.44
1:C:2583:ILE:HG23	1:C:2632:TYR:CE1	2.51	0.44
1:D:549:PHE:CE1	1:D:556:PRO:HB2	2.52	0.44
1:D:1201:LEU:HD22	1:D:1205:LEU:HB3	1.99	0.44
1:A:1514:PHE:CE1	1:B:1922:LEU:HD11	2.53	0.44
1:A:2189:TRP:HB3	1:A:2192:SER:OG	2.16	0.44
1:A:2555:ILE:HD11	1:A:2675:PHE:HB3	1.99	0.44
1:B:417:LEU:HD11	1:B:446:TRP:HB3	2.00	0.44
1:B:447:VAL:HG21	1:B:454:VAL:HG13	1.99	0.44
1:B:841:ILE:HA	1:B:871:VAL:HG12	1.98	0.44
1:B:1197:ARG:NH2	1:B:1198:THR:OG1	2.50	0.44
1:B:1473:GLU:O	1:B:1477:ASN:ND2	2.51	0.44
1:B:1475:LEU:HD22	1:B:1791:VAL:HG23	1.99	0.44
1:C:1464:PHE:HB3	1:C:1798:LEU:HD11	1.99	0.44
1:C:1697:ARG:HB3	1:D:2691:ILE:HG23	1.98	0.44
1:C:2085:LEU:O	1:C:2188:ARG:NH1	2.47	0.44
1:C:2568:PHE:CZ	1:C:2642:ARG:HD3	2.50	0.44
1:A:2752:ILE:HG12	1:A:2772:LEU:HB2	2.00	0.44
1:B:482:TYR:OH	1:B:752:ASP:O	2.21	0.44
1:B:2671:THR:HG23	1:B:2674:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:924:HIS:ND1	1:C:1110:ASP:HB3	2.32	0.44
1:D:411:HIS:CD2	1:D:414:ALA:HB2	2.51	0.44
1:A:37:HIS:HB3	1:A:39:PRO:HD2	2.00	0.44
1:A:1334:GLN:HA	1:A:1404:THR:HG21	2.00	0.44
1:A:1961:MET:HG3	1:A:2171:PRO:HB2	2.00	0.44
1:A:2044:LEU:HB2	1:A:2576:TYR:CD2	2.53	0.44
1:A:2094:CYS:HA	1:A:2097:VAL:HG12	1.99	0.44
1:A:2577:GLU:OE1	1:A:2580:ARG:NH1	2.50	0.44
1:A:2763:PRO:HG3	1:A:2775:PRO:HD2	1.98	0.44
1:B:38:PRO:HA	1:B:41:ASN:ND2	2.32	0.44
1:C:497:VAL:HG23	1:C:502:ARG:HG2	2.00	0.44
1:C:747:LEU:HD21	1:C:761:LYS:HB2	2.00	0.44
1:D:452:SER:HA	1:D:455:ALA:HB3	2.00	0.44
1:D:1078:SER:O	1:D:1082:LYS:HG2	2.17	0.44
1:D:1962:ASN:ND2	1:D:2180:ILE:O	2.48	0.44
1:A:1150:GLU:HA	1:A:1153:VAL:HG12	1.99	0.44
1:A:1922:LEU:HD11	1:B:1514:PHE:CE1	2.53	0.44
1:A:1934:ASP:HB2	1:B:1518:PRO:HB3	2.00	0.44
1:B:576:LEU:HD21	1:B:649:GLU:HB3	2.00	0.44
1:C:1408:GLU:OE1	1:C:1417:ARG:NH1	2.50	0.44
1:C:2598:MET:HG3	1:C:2599:ASP:N	2.32	0.44
1:D:12:PRO:HG3	1:D:861:LYS:HG2	2.00	0.44
1:D:397:GLU:HG2	1:D:399:GLU:H	1.81	0.44
1:D:423:LYS:HB2	1:D:423:LYS:HE3	1.76	0.44
1:D:747:LEU:HB2	1:D:759:VAL:HB	2.00	0.44
1:D:1252:LEU:HA	1:D:1255:LEU:HD12	1.99	0.44
1:D:2232:LEU:HG	1:D:2235:GLN:HE22	1.82	0.44
1:A:703:SER:O	1:A:707:ASP:HB2	2.17	0.44
1:A:876:LEU:HB2	1:A:891:TYR:CE2	2.53	0.44
1:A:2513:PHE:HD2	1:A:2551:ASN:HA	1.82	0.44
1:B:379:SER:OG	1:B:448:ASP:OD1	2.24	0.44
1:B:2727:GLN:HB3	1:B:2737:PRO:HB3	1.98	0.44
1:B:2728:ASP:HB3	1:B:2791:ILE:HB	1.99	0.44
1:C:66:ARG:HB3	1:C:362:TRP:CZ2	2.49	0.44
1:C:1124:ARG:NH2	1:C:1177:ASP:O	2.49	0.44
1:C:2595:PHE:HA	1:C:2598:MET:HG2	1.98	0.44
1:A:1777:TYR:HB2	1:B:1778:LEU:HD23	2.00	0.44
1:B:11:LEU:N	1:B:12:PRO:HD2	2.33	0.44
1:B:482:TYR:OH	1:B:755:GLY:O	2.36	0.44
1:B:874:GLN:NE2	1:B:877:MET:SD	2.91	0.44
1:B:2053:GLN:HB3	1:B:2055:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2730:VAL:HG12	1:B:2736:SER:O	2.17	0.44
1:C:2248:ARG:NH2	1:C:2308:LYS:O	2.51	0.44
1:D:49:LYS:HB2	1:D:63:GLU:HG3	2.00	0.44
1:D:890:GLN:HA	1:D:893:MET:HG2	1.98	0.44
1:D:1331:ARG:HA	1:D:1331:ARG:HD2	1.82	0.44
1:D:1365:PRO:O	1:D:1368:GLN:HG2	2.17	0.44
1:D:1929:ASN:O	1:D:1931:GLU:HG3	2.18	0.44
1:D:2256:MET:SD	1:D:2257:ARG:N	2.90	0.44
1:A:1206:CYS:N	1:A:1233:ASP:OD1	2.49	0.44
1:A:1231:TYR:HD1	1:A:1231:TYR:H	1.65	0.44
1:A:1340:LYS:HZ1	1:A:1420:GLU:HB3	1.83	0.44
1:A:1962:ASN:O	1:A:1965:THR:OG1	2.22	0.44
1:A:2602:PHE:CE2	1:A:2634:TYR:HB2	2.53	0.44
1:B:456:SER:H	1:B:457:LYS:HZ2	1.65	0.44
1:D:861:LYS:H	1:D:861:LYS:HD2	1.83	0.44
1:A:1125:ALA:HB1	1:A:1128:ALA:HB3	2.00	0.44
1:A:1856:GLY:HA3	1:B:1716:TRP:CZ2	2.53	0.44
1:B:532:THR:HG22	1:B:534:VAL:HG13	1.99	0.44
1:B:1868:PRO:HA	1:B:1873:HIS:CE1	2.53	0.44
1:B:2247:ASP:OD1	1:B:2251:LEU:N	2.50	0.44
1:C:2017:GLY:HA2	1:C:2632:TYR:HD2	1.83	0.44
1:D:915:ARG:NH1	1:D:919:ASN:OD1	2.51	0.44
1:D:2083:LYS:HG3	1:D:2188:ARG:NH1	2.33	0.44
1:A:1370:TYR:HE1	1:B:2088:VAL:HA	1.83	0.43
1:A:2201:MET:HE1	1:A:2212:LEU:HB3	1.99	0.43
1:A:2316:GLN:HG2	1:A:2317:ASN:H	1.83	0.43
1:A:2781:GLN:HA	1:A:2784:LYS:HZ3	1.83	0.43
1:B:1373:GLN:OE1	1:B:1374:GLN:NE2	2.50	0.43
1:B:1868:PRO:HA	1:B:1873:HIS:ND1	2.32	0.43
1:D:885:TYR:HA	1:D:1088:ILE:HD11	2.00	0.43
1:D:1387:LEU:HA	1:D:1391:CYS:SG	2.58	0.43
1:D:1813:ILE:HG22	1:D:1815:ALA:H	1.83	0.43
1:D:2240:LEU:HD23	1:D:2277:VAL:HG22	2.00	0.43
1:A:1439:LEU:HB3	1:A:1457:ILE:HD11	2.00	0.43
1:A:1499:LEU:HD12	1:A:1499:LEU:HA	1.89	0.43
1:B:1805:TYR:HE1	1:B:1809:VAL:HG11	1.83	0.43
1:B:1836:ILE:HG23	1:B:1837:PRO:HD3	1.99	0.43
1:C:817:GLY:O	1:C:841:ILE:N	2.42	0.43
1:C:925:ALA:O	1:C:929:VAL:HG22	2.17	0.43
1:C:1272:GLY:HA3	1:C:1354:LEU:HB2	2.00	0.43
1:D:390:LEU:HB3	1:D:411:HIS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1343:ILE:HG21	1:D:1424:VAL:HG13	2.00	0.43
1:A:747:LEU:HB3	1:A:799:VAL:HB	2.01	0.43
1:A:1194:PHE:CE1	1:A:1223:LEU:HB2	2.54	0.43
1:A:2690:LEU:O	1:A:2694:THR:OG1	2.31	0.43
1:B:75:GLN:HB2	1:B:77:ASP:OD1	2.18	0.43
1:B:1124:ARG:NH2	1:B:1176:ASN:O	2.52	0.43
1:B:1784:LEU:HD12	1:B:1784:LEU:HA	1.87	0.43
1:B:2183:ASP:OD1	1:B:2184:MET:N	2.51	0.43
1:C:381:LEU:HG	1:C:382:LEU:N	2.34	0.43
1:C:917:ASP:N	1:C:917:ASP:OD1	2.50	0.43
1:C:2763:PRO:HG3	1:C:2775:PRO:HD3	2.00	0.43
1:D:443:VAL:HG21	1:D:494:TRP:HZ2	1.82	0.43
1:D:471:GLU:HB2	1:D:487:LEU:HD23	2.00	0.43
1:D:844:LEU:HD12	1:D:845:GLY:N	2.33	0.43
1:D:1961:MET:O	1:D:1965:THR:HG23	2.18	0.43
1:D:2272:MET:SD	1:D:2272:MET:N	2.84	0.43
1:D:2571:PHE:CE2	1:D:2642:ARG:HD3	2.53	0.43
1:A:478:CYS:HA	1:A:483:THR:HA	2.00	0.43
1:A:1834:LYS:HD3	1:A:1834:LYS:HA	1.92	0.43
1:A:2515:THR:HG22	1:A:2551:ASN:HB2	2.00	0.43
1:C:662:VAL:HB	1:C:663:LYS:HD3	1.99	0.43
1:C:1120:ALA:HA	1:C:1125:ALA:HB3	1.99	0.43
1:D:877:MET:O	1:D:880:ILE:HG13	2.19	0.43
1:A:52:VAL:HB	1:A:376:ALA:HB2	2.00	0.43
1:A:682:PHE:HD2	1:A:709:ARG:HG3	1.83	0.43
1:A:922:ILE:HG13	1:A:923:LEU:HD22	2.01	0.43
1:A:2616:GLU:OE1	1:A:2621:GLY:N	2.42	0.43
1:B:497:VAL:HG12	1:B:498:PRO:HD2	2.01	0.43
1:B:2633:GLU:O	1:B:2637:LYS:HG2	2.18	0.43
1:C:76:PRO:HB3	1:C:851:LEU:HD22	2.00	0.43
1:C:1411:ASN:HB3	1:C:1418:ARG:NH1	2.34	0.43
1:D:21:ARG:O	1:D:25:VAL:HG23	2.18	0.43
1:D:924:HIS:CD2	1:D:1110:ASP:HB3	2.53	0.43
1:D:1937:PRO:HB2	1:D:1939:LEU:HD22	2.00	0.43
1:D:2075:TYR:HB2	1:D:2086:MET:HE3	2.00	0.43
1:A:68:CYS:SG	1:A:69:ARG:N	2.91	0.43
1:A:492:TYR:CD1	1:A:737:LYS:HA	2.53	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD23	1.73	0.43
1:B:38:PRO:N	1:B:39:PRO:HD2	2.33	0.43
1:B:533:GLN:HA	1:B:668:GLY:C	2.38	0.43
1:B:2221:LYS:HD2	1:B:2674:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2595:PHE:CG	1:B:2628:PRO:HG3	2.54	0.43
1:C:491:LEU:HB2	1:C:738:LEU:HB2	2.00	0.43
1:C:1787:ALA:O	1:C:1791:VAL:HG23	2.19	0.43
1:D:37:HIS:HE2	1:D:352:SER:HG	1.66	0.43
1:D:838:LEU:HD21	1:D:841:ILE:HD11	2.01	0.43
1:A:1110:ASP:OD1	1:A:1111:ALA:N	2.52	0.43
1:A:1196:CYS:SG	1:A:1198:THR:OG1	2.76	0.43
1:B:377:LEU:HD21	1:B:432:ILE:O	2.19	0.43
1:B:479:CYS:HB3	1:B:751:VAL:CG1	2.48	0.43
1:B:2714:PHE:O	1:B:2717:ILE:HG13	2.18	0.43
1:C:1438:ILE:HD12	1:D:1918:LEU:HD22	2.01	0.43
1:C:2088:VAL:HG12	1:D:1373:GLN:CD	2.38	0.43
1:D:541:LEU:O	1:D:565:VAL:N	2.52	0.43
1:D:749:VAL:HG12	1:D:758:ALA:HA	2.01	0.43
1:B:895:LEU:HD11	1:B:908:LEU:HD13	1.99	0.43
1:C:23:ARG:NH1	1:C:27:GLU:OE2	2.52	0.43
1:C:790:ALA:HB1	1:C:919:ASN:HB2	2.00	0.43
1:C:2199:VAL:HG13	1:D:1707:ALA:HA	2.00	0.43
1:C:2575:MET:HE3	1:C:2579:LEU:HD13	1.99	0.43
1:C:2607:CYS:SG	1:C:2608:LYS:N	2.92	0.43
1:C:2766:ASN:O	1:C:2770:SER:CA	2.67	0.43
1:D:561:LEU:HD21	1:D:572:CYS:SG	2.59	0.43
1:D:819:ILE:HD12	1:D:819:ILE:HA	1.88	0.43
1:D:1485:PRO:O	1:D:1489:GLY:N	2.49	0.43
1:D:2074:LEU:HB3	1:D:2086:MET:HB3	2.00	0.43
1:A:1340:LYS:NZ	1:A:1420:GLU:HB3	2.34	0.43
1:A:1691:LEU:HB2	1:B:2712:ARG:HH12	1.84	0.43
1:A:1854:ARG:HE	1:A:2191:LEU:HD13	1.83	0.43
1:A:1924:LEU:HD13	1:B:1485:PRO:HG3	2.00	0.43
1:A:2708:LEU:HA	1:A:2711:LYS:HG2	2.00	0.43
1:B:401:TYR:HD2	1:B:410:HIS:HD2	1.67	0.43
1:B:1155:MET:HA	1:B:1158:VAL:HG12	2.01	0.43
1:B:2182:HIS:O	1:B:2186:LEU:HG	2.18	0.43
1:C:2714:PHE:O	1:C:2717:ILE:HG13	2.18	0.43
1:D:920:ARG:HB3	1:D:924:HIS:HB3	2.01	0.43
1:D:1962:ASN:O	1:D:1965:THR:OG1	2.22	0.43
1:D:2655:ARG:CZ	1:D:2659:LEU:HD11	2.49	0.43
1:A:2239:ASP:OD1	1:A:2275:HIS:HB3	2.19	0.43
1:A:2297:THR:HG22	1:A:2301:GLN:OE1	2.19	0.43
1:B:655:GLU:N	1:B:655:GLU:OE1	2.52	0.43
1:B:1197:ARG:HE	1:B:1220:ASP:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1940:ASP:OD1	1:B:1940:ASP:N	2.52	0.43
1:B:2552:ARG:NH1	1:B:2556:LYS:HG3	2.34	0.43
1:B:2721:MET:HB2	1:B:2725:GLU:HG3	2.01	0.43
1:C:1917:PHE:HB2	1:D:1494:THR:HG21	2.00	0.43
1:C:2203:ASP:OD1	1:C:2204:VAL:HG23	2.19	0.43
1:D:479:CYS:HB3	1:D:751:VAL:HG12	2.00	0.43
1:D:761:LYS:NZ	1:D:763:GLY:O	2.41	0.43
1:D:1839:TRP:CE3	1:D:1954:LEU:HD13	2.52	0.43
1:D:2182:HIS:O	1:D:2186:LEU:HG	2.19	0.43
1:A:451:LEU:O	1:A:454:VAL:HG22	2.19	0.42
1:A:813:ARG:HH12	1:A:842:SER:C	2.22	0.42
1:A:1366:GLU:O	1:A:1369:VAL:HG12	2.18	0.42
1:A:1520:PRO:HG2	1:B:1864:ASP:HB3	2.01	0.42
1:A:2252:ILE:O	1:A:2256:MET:HG2	2.19	0.42
1:B:876:LEU:HD23	1:B:911:PHE:CE1	2.54	0.42
1:B:2253:GLN:HE21	1:B:2310:PRO:HB2	1.84	0.42
1:C:509:ALA:O	1:C:513:ASN:N	2.43	0.42
1:C:2219:GLU:O	1:C:2222:GLU:HG3	2.18	0.42
1:D:403:ASN:HB3	1:D:406:ASN:O	2.19	0.42
1:D:569:ASN:N	1:D:569:ASN:OD1	2.52	0.42
1:D:2558:LEU:HD23	1:D:2655:ARG:HA	2.00	0.42
1:A:70:ILE:HD11	1:A:357:GLY:HA3	2.00	0.42
1:A:711:LEU:HD13	1:A:716:LEU:HD11	2.01	0.42
1:A:1226:THR:O	1:A:1228:PRO:HD3	2.19	0.42
1:B:877:MET:HE3	1:B:914:HIS:HB3	2.00	0.42
1:C:1481:SER:HB2	1:D:1928:HIS:ND1	2.34	0.42
1:C:2552:ARG:HD3	1:C:2570:PHE:CG	2.54	0.42
1:D:565:VAL:HA	1:D:572:CYS:SG	2.59	0.42
1:D:655:GLU:N	1:D:655:GLU:OE1	2.52	0.42
1:D:770:ILE:O	1:D:779:GLU:HG3	2.19	0.42
1:D:1117:PHE:CE1	1:D:1129:ALA:HB1	2.54	0.42
1:D:1714:MET:HA	1:D:1716:TRP:CD1	2.55	0.42
1:D:1852:GLN:HE22	1:D:1939:LEU:HB3	1.83	0.42
1:A:687:SER:HB3	1:A:706:GLN:HB3	2.01	0.42
1:B:560:VAL:HG13	1:B:575:GLN:HB3	2.01	0.42
1:B:705:LEU:HD21	1:D:671:LEU:HD13	2.00	0.42
1:B:1871:PRO:HG3	1:B:1936:LEU:HD21	1.99	0.42
1:B:2223:SER:O	1:B:2227:ARG:HG2	2.19	0.42
1:B:2710:PHE:HE1	1:B:2777:TYR:HB2	1.85	0.42
1:B:2766:ASN:O	1:B:2770:SER:CA	2.68	0.42
1:C:2050:LEU:HD13	1:C:2066:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:ARG:HB3	1:D:514:LYS:HB3	2.02	0.42
1:D:549:PHE:CG	1:D:550:SER:N	2.87	0.42
1:D:1180:SER:HA	1:D:1183:TRP:HE1	1.85	0.42
1:A:443:VAL:HG12	1:A:476:LEU:HD11	2.02	0.42
1:A:1475:LEU:HA	1:A:1478:VAL:HG12	2.02	0.42
1:A:2230:GLU:HA	1:A:2233:ARG:HG2	2.00	0.42
1:B:22:LEU:HD13	1:B:819:ILE:HG12	2.02	0.42
1:B:1402:LEU:HD13	1:B:1466:ALA:HB3	2.01	0.42
1:C:1125:ALA:HB1	1:C:1128:ALA:HB3	2.02	0.42
1:C:1269:ASN:HD21	1:C:1273:GLU:HG3	1.83	0.42
1:C:1707:ALA:HB1	1:C:1718:VAL:HG12	2.01	0.42
1:C:1955:ILE:HD13	1:C:1958:ILE:HD12	2.01	0.42
1:B:562:MET:N	1:B:562:MET:SD	2.92	0.42
1:B:1164:ASN:N	1:B:1164:ASN:OD1	2.52	0.42
1:C:1170:LEU:HD12	1:C:1170:LEU:HA	1.82	0.42
1:C:1475:LEU:HD22	1:C:1791:VAL:HG13	2.02	0.42
1:C:2519:GLY:H	1:C:2525:ARG:CZ	2.32	0.42
1:C:2554:VAL:HA	1:C:2557:VAL:HG22	2.02	0.42
1:D:1092:LEU:O	1:D:1095:SER:OG	2.31	0.42
1:D:1102:LEU:HD23	1:D:1105:LEU:HD12	2.01	0.42
1:D:2083:LYS:HG3	1:D:2188:ARG:HH11	1.84	0.42
1:A:1197:ARG:NH2	1:A:1202:LEU:HB2	2.35	0.42
1:A:1791:VAL:O	1:A:1795:ILE:HG23	2.20	0.42
1:A:2763:PRO:HB3	1:A:2774:VAL:HG12	2.01	0.42
1:B:1115:THR:OG1	1:B:1118:MET:HG3	2.20	0.42
1:B:1170:LEU:HB2	1:B:1264:LEU:HD23	2.02	0.42
1:C:352:SER:HA	1:C:353:PRO:HD3	1.85	0.42
1:C:726:LYS:O	1:C:727:VAL:HB	2.18	0.42
1:C:752:ASP:HB3	1:C:803:THR:HG21	2.02	0.42
1:D:2595:PHE:CD1	1:D:2600:LEU:HB2	2.55	0.42
1:D:2671:THR:OG1	1:D:2672:ALA:N	2.53	0.42
1:A:385:SER:HB3	1:A:391:TYR:HE2	1.84	0.42
1:A:492:TYR:HD1	1:A:737:LYS:HA	1.85	0.42
1:A:2102:MET:SD	1:A:2103:SER:N	2.92	0.42
1:A:2534:ARG:HH11	1:A:2660:ASP:HB2	1.85	0.42
1:B:497:VAL:HG23	1:B:730:CYS:O	2.19	0.42
1:C:442:LYS:HB3	1:C:462:ALA:HB1	2.00	0.42
1:C:1117:PHE:CE1	1:C:1129:ALA:HB1	2.55	0.42
1:C:1177:ASP:H	1:C:1251:ARG:HH22	1.67	0.42
1:C:1331:ARG:O	1:C:1331:ARG:NH1	2.53	0.42
1:C:1941:VAL:HG21	1:C:2195:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2721:MET:HE1	1:C:2729:LEU:HB2	2.02	0.42
1:D:2532:ILE:O	1:D:2535:ILE:HG12	2.19	0.42
1:A:551:ILE:HA	1:A:556:PRO:HA	2.01	0.42
1:A:667:VAL:O	1:A:669:LYS:NZ	2.39	0.42
1:A:1402:LEU:HD11	1:A:1463:VAL:HA	2.01	0.42
1:A:1500:ALA:HB1	1:A:1505:ASP:HB3	2.01	0.42
1:A:1828:GLN:HB2	1:A:2169:PHE:HZ	1.84	0.42
1:A:2294:SER:OG	1:A:2735:SER:HB2	2.19	0.42
1:A:2715:TRP:HA	1:A:2718:VAL:HG22	2.01	0.42
1:B:804:ALA:HB2	1:B:846:MET:HG2	2.02	0.42
1:C:432:ILE:HG21	1:C:551:ILE:HD12	2.00	0.42
1:C:501:GLN:HA	1:C:504:LYS:HG2	2.00	0.42
1:D:380:GLU:HA	1:D:394:LYS:HA	2.01	0.42
1:D:1362:HIS:CD2	1:D:1362:HIS:H	2.36	0.42
1:D:2784:LYS:O	1:D:2787:LEU:HG	2.20	0.42
1:A:536:LEU:HD23	1:A:716:LEU:HG	2.01	0.42
1:A:881:LEU:HA	1:A:929:VAL:HG11	2.02	0.42
1:A:893:MET:O	1:A:896:GLU:HG3	2.19	0.42
1:A:1266:THR:HA	1:A:1274:HIS:HE1	1.85	0.42
1:A:1927:SER:OG	1:A:2090:VAL:HG13	2.19	0.42
1:A:2792:LYS:HB3	1:A:2792:LYS:HE3	1.83	0.42
1:B:1235:TRP:CE3	1:B:1315:PRO:HD3	2.54	0.42
1:B:1259:LEU:HD11	1:B:1332:VAL:HG22	2.01	0.42
1:B:1470:TYR:HA	1:B:1473:GLU:HG3	2.02	0.42
1:C:427:LEU:HD23	1:C:428:SER:N	2.34	0.42
1:C:885:TYR:CZ	1:C:1087:PHE:HB3	2.55	0.42
1:C:1917:PHE:CE2	1:D:1441:VAL:HG11	2.41	0.42
1:C:2605:ASP:OD1	1:C:2605:ASP:N	2.45	0.42
1:A:679:ALA:HB2	1:C:710:LEU:HD11	2.02	0.42
1:A:1102:LEU:HA	1:A:1105:LEU:HB2	2.01	0.42
1:A:1367:GLU:OE1	1:A:1367:GLU:N	2.53	0.42
1:A:1842:MET:SD	1:A:1951:PHE:HA	2.60	0.42
1:A:2064:GLU:HG2	1:A:2190:ARG:HH12	1.85	0.42
1:A:2766:ASN:HD21	1:A:2773:TYR:HE2	1.66	0.42
1:B:745:GLU:N	1:B:745:GLU:OE1	2.53	0.42
1:B:1124:ARG:NH1	1:B:1244:ILE:O	2.53	0.42
1:B:2572:ASP:OD1	1:B:2572:ASP:N	2.52	0.42
1:C:1348:GLN:NE2	1:C:1372:ASN:O	2.53	0.42
1:C:1386:CYS:HA	1:C:1390:LYS:HG2	2.02	0.42
1:C:2229:MET:HA	1:C:2232:LEU:HG	2.01	0.42
1:D:377:LEU:HD11	1:D:382:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:LYS:HE2	1:D:457:LYS:HB3	1.87	0.42
1:D:1476:CYS:SG	1:D:1831:VAL:HG23	2.60	0.42
1:D:1846:MET:HA	1:D:1849:THR:HG22	2.01	0.42
1:A:69:ARG:NH1	1:A:395:TRP:HA	2.35	0.41
1:A:1201:LEU:HD21	1:A:1234:CYS:HA	2.02	0.41
1:A:2763:PRO:CA	1:A:2773:TYR:O	2.68	0.41
1:B:2232:LEU:O	1:B:2235:GLN:NE2	2.38	0.41
1:C:74:VAL:HG12	1:C:849:HIS:ND1	2.34	0.41
1:C:1513:LEU:HD21	1:D:1919:ASN:HA	2.02	0.41
1:D:11:LEU:N	1:D:12:PRO:HD2	2.34	0.41
1:D:1709:GLN:OE1	1:D:1709:GLN:N	2.47	0.41
1:A:2580:ARG:NH1	1:A:2581:GLN:OE1	2.52	0.41
1:A:2726:ARG:O	1:A:2730:VAL:HG23	2.20	0.41
1:B:710:LEU:HD11	1:D:679:ALA:HB2	2.01	0.41
1:B:1364:LEU:O	1:B:1368:GLN:HG3	2.20	0.41
1:B:2552:ARG:HH11	1:B:2556:LYS:HG3	1.85	0.41
1:C:22:LEU:O	1:C:25:VAL:HG12	2.19	0.41
1:C:441:ASN:ND2	1:C:441:ASN:O	2.53	0.41
1:C:750:ASN:OD1	1:C:803:THR:N	2.52	0.41
1:C:840:PRO:O	1:C:872:GLU:N	2.41	0.41
1:C:1716:TRP:CZ2	1:D:1856:GLY:HA3	2.54	0.41
1:C:2788:LEU:HD13	1:C:2791:ILE:HD11	2.01	0.41
1:D:1776:SER:O	1:D:1779:THR:HG22	2.20	0.41
1:D:2097:VAL:HB	1:D:2101:LYS:HE3	2.00	0.41
1:A:493:TRP:CD1	1:A:736:LYS:HB3	2.54	0.41
1:B:463:GLN:HB3	1:B:465:TYR:CE1	2.55	0.41
1:B:846:MET:HA	1:B:866:VAL:O	2.21	0.41
1:C:1336:TRP:CD1	1:C:1408:GLU:HG3	2.54	0.41
1:C:2265:ARG:HD3	1:C:2266:ARG:H	1.85	0.41
1:D:381:LEU:HB2	1:D:395:TRP:CH2	2.55	0.41
1:D:440:ASN:HB3	1:D:442:LYS:HE2	2.02	0.41
1:D:2554:VAL:HG13	1:D:2651:LEU:HD11	2.01	0.41
1:A:908:LEU:O	1:A:912:ILE:HG12	2.19	0.41
1:A:1871:PRO:HB3	1:B:1716:TRP:CD1	2.55	0.41
1:B:1179:CYS:O	1:B:1182:THR:OG1	2.35	0.41
1:B:2058:GLN:OE1	1:B:2060:ASN:N	2.39	0.41
1:C:381:LEU:HG	1:C:382:LEU:H	1.86	0.41
1:D:2730:VAL:HA	1:D:2733:TRP:HB2	2.03	0.41
1:A:2600:LEU:O	1:A:2626:VAL:N	2.54	0.41
1:B:1099:GLN:OE1	1:B:1099:GLN:N	2.54	0.41
1:B:1438:ILE:HD13	1:B:1438:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2556:LYS:HD3	1:B:2556:LYS:HA	1.90	0.41
1:C:502:ARG:NH1	1:C:657:VAL:HA	2.36	0.41
1:C:784:PHE:HD2	1:C:820:TYR:CZ	2.38	0.41
1:C:1156:GLY:HA2	1:C:1160:PRO:HA	2.02	0.41
1:C:1716:TRP:CE3	1:D:1936:LEU:HD13	2.55	0.41
1:C:1936:LEU:HD12	1:C:1936:LEU:HA	1.94	0.41
1:D:432:ILE:HD12	1:D:451:LEU:HD11	2.02	0.41
1:D:542:TYR:HB3	1:D:564:SER:HA	2.03	0.41
1:D:543:HIS:CB	1:D:665:VAL:HG11	2.48	0.41
1:D:1102:LEU:HD23	1:D:1102:LEU:HA	1.91	0.41
1:D:1834:LYS:HA	1:D:1834:LYS:HD3	1.76	0.41
1:D:2269:THR:OG1	1:D:2270:THR:N	2.51	0.41
1:A:1259:LEU:HD21	1:A:1332:VAL:HG22	2.02	0.41
1:B:1340:LYS:O	1:B:1344:MET:HB2	2.20	0.41
1:C:1169:PRO:HD2	1:C:1264:LEU:HD13	2.01	0.41
1:C:1339:LEU:HA	1:C:1339:LEU:HD22	1.86	0.41
1:C:1403:GLY:O	1:C:1407:LYS:HG2	2.21	0.41
1:C:1821:TYR:CE1	1:C:2164:PRO:HB2	2.55	0.41
1:C:1941:VAL:HG13	1:C:2196:PHE:HE1	1.86	0.41
1:D:68:CYS:SG	1:D:69:ARG:N	2.94	0.41
1:A:495:GLY:O	1:A:732:GLN:HB3	2.20	0.41
1:B:1179:CYS:SG	1:B:1180:SER:N	2.93	0.41
1:C:441:ASN:O	1:C:464:THR:OG1	2.39	0.41
1:C:1187:GLU:H	1:C:1187:GLU:HG3	1.71	0.41
1:D:757:HIS:NE2	1:D:810:ILE:HG13	2.36	0.41
1:A:2087:GLU:OE2	1:A:2188:ARG:HG2	2.21	0.41
1:B:896:GLU:OE2	1:B:897:GLN:NE2	2.53	0.41
1:B:1201:LEU:HD22	1:B:1205:LEU:HB3	2.03	0.41
1:C:8:VAL:HG12	1:C:866:VAL:HG22	2.01	0.41
1:C:851:LEU:HD12	1:C:851:LEU:H	1.85	0.41
1:C:917:ASP:O	1:C:920:ARG:HG3	2.20	0.41
1:C:1170:LEU:HD11	1:C:1255:LEU:HD12	2.03	0.41
1:C:2238:ARG:HD3	1:C:2238:ARG:HA	1.89	0.41
1:D:1114:MET:HB3	1:D:1118:MET:HB2	2.03	0.41
1:D:2247:ASP:OD1	1:D:2251:LEU:N	2.54	0.41
1:D:2257:ARG:NH2	1:D:2314:CYS:SG	2.94	0.41
1:A:63:GLU:OE1	1:A:63:GLU:N	2.54	0.41
1:A:813:ARG:NH1	1:A:842:SER:O	2.41	0.41
1:A:917:ASP:OD1	1:A:917:ASP:N	2.54	0.41
1:A:921:ASN:ND2	1:A:1108:ALA:HB3	2.36	0.41
1:A:1089:LEU:HD13	1:A:1089:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:HIS:O	1:A:1317:HIS:ND1	2.52	0.41
1:A:1376:GLY:O	1:A:1427:ARG:NH2	2.44	0.41
1:A:1492:ARG:HG3	1:B:1940:ASP:OD2	2.21	0.41
1:A:2186:LEU:HD22	1:A:2193:LEU:HD11	2.03	0.41
1:A:2257:ARG:HA	1:A:2257:ARG:NH1	2.36	0.41
1:A:2601:ALA:HA	1:A:2625:PRO:HA	2.03	0.41
1:B:5:HIS:CE1	1:B:29:LEU:HD13	2.56	0.41
1:B:514:LYS:O	1:B:515:LYS:HG2	2.21	0.41
1:B:710:LEU:HD22	1:D:710:LEU:HD13	2.02	0.41
1:B:1431:SER:HA	1:B:1434:ARG:CZ	2.50	0.41
1:B:1480:GLU:HA	1:B:1483:ILE:HG22	2.03	0.41
1:B:2185:LEU:HD12	1:B:2189:TRP:CZ3	2.56	0.41
1:C:880:ILE:HA	1:C:1088:ILE:HD13	2.02	0.41
1:C:1189:ILE:HD13	1:C:1189:ILE:HA	1.82	0.41
1:C:1329:LEU:HA	1:C:1332:VAL:HG12	2.02	0.41
1:C:1404:THR:O	1:C:1408:GLU:HG2	2.21	0.41
1:C:2519:GLY:H	1:C:2525:ARG:NH2	2.17	0.41
1:C:2564:ASN:ND2	1:C:2567:ASP:OD1	2.53	0.41
1:D:40:LEU:O	1:D:44:GLU:HG2	2.20	0.41
1:D:413:ARG:O	1:D:417:LEU:HG	2.21	0.41
1:D:1819:LEU:O	1:D:2166:LEU:HD11	2.20	0.41
1:D:2649:GLN:CD	1:D:2649:GLN:H	2.23	0.41
1:A:433:ARG:HH12	1:A:495:GLY:CA	2.33	0.41
1:B:2564:ASN:N	1:B:2567:ASP:OD2	2.44	0.41
1:C:49:LYS:HD2	1:C:49:LYS:HA	1.81	0.41
1:C:401:TYR:CE1	1:C:410:HIS:HA	2.56	0.41
1:C:530:VAL:HG22	1:C:673:VAL:HB	2.03	0.41
1:C:751:VAL:O	1:C:805:GLY:HA2	2.20	0.41
1:D:1478:VAL:O	1:D:1481:SER:OG	2.23	0.41
1:A:69:ARG:HD2	1:A:395:TRP:CE3	2.57	0.40
1:A:490:SER:HB3	1:A:492:TYR:CZ	2.56	0.40
1:A:2766:ASN:OD1	1:A:2766:ASN:N	2.50	0.40
1:B:424:ILE:HG23	1:B:436:VAL:HG13	2.03	0.40
1:B:515:LYS:O	1:B:517:LYS:HD3	2.21	0.40
1:B:852:ILE:H	1:B:852:ILE:HG13	1.64	0.40
1:B:2185:LEU:HD13	1:B:2185:LEU:HA	1.84	0.40
1:B:2269:THR:OG1	1:B:2270:THR:N	2.54	0.40
1:C:377:LEU:HA	1:C:430:ASN:O	2.21	0.40
1:C:753:SER:HB3	1:C:806:GLN:HA	2.02	0.40
1:C:766:VAL:HG11	1:C:791:PHE:CD2	2.56	0.40
1:C:1187:GLU:OE1	1:C:1189:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2699:GLU:OE2	1:C:2755:ARG:NE	2.50	0.40
1:D:732:GLN:NE2	1:D:734:THR:O	2.53	0.40
1:D:1355:SER:HB3	1:D:1358:SER:HB2	2.03	0.40
1:D:1480:GLU:O	1:D:1484:VAL:HG23	2.21	0.40
1:D:2505:PHE:HD1	1:D:2516:PRO:HA	1.85	0.40
1:A:411:HIS:O	1:A:413:ARG:N	2.53	0.40
1:A:474:VAL:HB	1:A:486:GLN:O	2.21	0.40
1:A:2504:LEU:HA	1:A:2525:ARG:NH2	2.36	0.40
1:A:2790:ALA:O	1:A:2793:THR:OG1	2.33	0.40
1:B:19:ASN:ND2	1:B:822:MET:O	2.50	0.40
1:B:672:LYS:HB3	1:B:679:ALA:HB3	2.03	0.40
1:B:1102:LEU:HD23	1:B:1102:LEU:HA	1.89	0.40
1:B:1235:TRP:CZ2	1:B:1314:MET:HG3	2.56	0.40
1:B:2225:PHE:O	1:B:2229:MET:HG2	2.21	0.40
1:C:2026:SER:OG	1:C:2027:ASP:N	2.54	0.40
1:C:2199:VAL:HG22	1:D:1710:ALA:HB2	2.03	0.40
1:C:2667:LEU:HA	1:C:2670:LEU:HD12	2.03	0.40
1:D:75:GLN:NE2	1:D:353:PRO:O	2.45	0.40
1:D:494:TRP:HB3	1:D:735:PRO:HA	2.02	0.40
1:D:923:LEU:HD22	1:D:1092:LEU:HD21	2.04	0.40
1:D:1345:PHE:CE1	1:D:1352:ASP:HB3	2.56	0.40
1:D:1345:PHE:CZ	1:D:1352:ASP:HB3	2.56	0.40
1:D:2757:PRO:HD3	1:D:2776:LEU:HB3	2.02	0.40
1:A:502:ARG:O	1:A:505:MET:HG3	2.21	0.40
1:A:529:THR:O	1:A:532:THR:OG1	2.35	0.40
1:A:1961:MET:O	1:A:1965:THR:HG23	2.22	0.40
1:A:2059:PRO:HA	1:A:2677:LEU:HD21	2.03	0.40
1:B:373:CYS:SG	1:B:427:LEU:HB3	2.62	0.40
1:B:517:LYS:HB2	1:B:517:LYS:HE2	1.83	0.40
1:B:827:MET:HB2	1:B:1197:ARG:NH1	2.36	0.40
1:B:924:HIS:ND1	1:B:1110:ASP:HB3	2.37	0.40
1:B:2095:LEU:HD12	1:B:2095:LEU:HA	1.82	0.40
1:C:386:SER:O	1:C:423:LYS:NZ	2.37	0.40
1:C:787:SER:OG	1:C:1111:ALA:O	2.33	0.40
1:C:1202:LEU:N	1:C:1205:LEU:HB2	2.36	0.40
1:C:1422:ILE:O	1:C:1426:MET:HG2	2.22	0.40
1:C:2225:PHE:O	1:C:2228:GLU:HG3	2.22	0.40
1:D:444:ALA:HB2	1:D:462:ALA:HB2	2.04	0.40
1:D:1233:ASP:OD1	1:D:1233:ASP:N	2.44	0.40
1:D:2530:ARG:NH2	1:D:2657:GLY:HA2	2.37	0.40
1:A:2256:MET:SD	1:A:2531:ASN:ND2	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2700:SER:HB3	1:A:2756:PRO:HA	2.03	0.40
1:B:433:ARG:HD2	1:B:483:THR:OG1	2.22	0.40
1:B:2079:ALA:HB1	1:B:2084:CYS:HB3	2.02	0.40
1:C:11:LEU:HA	1:C:11:LEU:HD23	1.83	0.40
1:C:68:CYS:SG	1:C:69:ARG:N	2.95	0.40
1:C:1240:CYS:SG	1:C:1242:THR:OG1	2.76	0.40
1:C:1436:PHE:HB2	1:C:1460:CYS:SG	2.62	0.40
1:C:1854:ARG:NH1	1:D:1370:TYR:OH	2.46	0.40
1:C:2288:GLY:O	1:C:2291:VAL:HG12	2.21	0.40
1:C:2677:LEU:HA	1:C:2677:LEU:HD12	1.84	0.40
1:D:925:ALA:HA	1:D:928:SER:HB3	2.03	0.40
1:D:1295:PRO:HA	1:D:1296:PRO:HD3	1.88	0.40
1:A:433:ARG:NH1	1:A:482:TYR:HA	2.37	0.40
1:A:562:MET:H	1:A:562:MET:HG3	1.62	0.40
1:A:574:PHE:HD2	1:A:651:TRP:HB2	1.87	0.40
1:A:1483:ILE:HD12	1:A:1483:ILE:HA	1.93	0.40
1:A:1841:TRP:HZ3	1:A:1950:VAL:HG21	1.86	0.40
1:A:2240:LEU:HD23	1:A:2274:VAL:HG11	2.03	0.40
1:B:785:PRO:HG3	1:B:831:ARG:O	2.21	0.40
1:B:888:CYS:SG	1:B:889:ARG:N	2.94	0.40
1:B:1432:VAL:HA	1:B:1435:VAL:HG12	2.03	0.40
1:C:752:ASP:HA	1:C:805:GLY:HA2	2.04	0.40
1:C:872:GLU:N	1:C:872:GLU:OE1	2.54	0.40
1:C:2228:GLU:O	1:C:2232:LEU:HG	2.21	0.40
1:C:2685:VAL:HG13	1:C:2739:LEU:HD12	2.03	0.40
1:D:6:PHE:HD1	1:D:868:ILE:HG22	1.86	0.40
1:D:483:THR:O	1:D:493:TRP:HA	2.21	0.40
1:D:1280:VAL:HG21	1:D:1383:PHE:CD1	2.56	0.40
1:D:1799:MET:HE1	1:D:1831:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1753/2799 (63%)	1658 (95%)	94 (5%)	1 (0%)	51	84
1	B	1753/2799 (63%)	1654 (94%)	97 (6%)	2 (0%)	51	84
1	C	1753/2799 (63%)	1658 (95%)	93 (5%)	2 (0%)	51	84
1	D	1753/2799 (63%)	1635 (93%)	117 (7%)	1 (0%)	51	84
All	All	7012/11196 (63%)	6605 (94%)	401 (6%)	6 (0%)	54	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	727	VAL
1	B	515	LYS
1	B	2088	VAL
1	D	542	TYR
1	A	662	VAL
1	C	2088	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1561/2419 (64%)	1488 (95%)	73 (5%)	26	60
1	B	1561/2419 (64%)	1488 (95%)	73 (5%)	26	60
1	C	1561/2419 (64%)	1485 (95%)	76 (5%)	25	59
1	D	1561/2419 (64%)	1481 (95%)	80 (5%)	24	57
All	All	6244/9676 (64%)	5942 (95%)	302 (5%)	29	60

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	7	VAL
1	A	8	VAL
1	A	18	LEU
1	A	60	PHE

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Mol	Chain	Res	Type
1	A	377	LEU
1	A	411	HIS
1	A	461	THR
1	A	501	GLN
1	A	541	LEU
1	A	650	GLN
1	A	654	ARG
1	A	681	LYS
1	A	762	THR
1	A	767	ARG
1	A	784	PHE
1	A	803	THR
1	A	806	GLN
1	A	836	LEU
1	A	849	HIS
1	A	854	LEU
1	A	872	GLU
1	A	1110	ASP
1	A	1153	VAL
1	A	1164	ASN
1	A	1209	THR
1	A	1225	ARG
1	A	1231	TYR
1	A	1238	CYS
1	A	1262	THR
1	A	1267	LEU
1	A	1367	GLU
1	A	1389	VAL
1	A	1396	LEU
1	A	1405	LEU
1	A	1409	LEU
1	A	1439	LEU
1	A	1441	VAL
1	A	1480	GLU
1	A	1490	ILE
1	A	1513	LEU
1	A	1517	GLU
1	A	1522	ARG
1	A	1823	ASP
1	A	1846	MET
1	A	1922	LEU
1	A	1929	ASN

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Mol	Chain	Res	Type
1	A	1932	HIS
1	A	1939	LEU
1	A	1961	MET
1	A	2041	GLU
1	A	2042	VAL
1	A	2089	THR
1	A	2095	LEU
1	A	2102	MET
1	A	2194	GLU
1	A	2201	MET
1	A	2204	VAL
1	A	2240	LEU
1	A	2242	LEU
1	A	2253	GLN
1	A	2269	THR
1	A	2539	CYS
1	A	2540	LEU
1	A	2548	ILE
1	A	2554	VAL
1	A	2572	ASP
1	A	2581	GLN
1	A	2623	ASN
1	A	2721	MET
1	A	2731	TYR
1	A	2746	PHE
1	A	2766	ASN
1	B	9	HIS
1	B	11	LEU
1	B	75	GLN
1	B	377	LEU
1	B	390	LEU
1	B	436	VAL
1	B	473	ILE
1	B	476	LEU
1	B	479	CYS
1	B	501	GLN
1	B	507	GLU
1	B	534	VAL
1	B	542	TYR
1	B	551	ILE
1	B	563	GLU
1	B	724	THR

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Mol	Chain	Res	Type
1	B	726	LYS
1	B	756	VAL
1	B	818	THR
1	B	849	HIS
1	B	880	ILE
1	B	888	CYS
1	B	911	PHE
1	B	914	HIS
1	B	916	CYS
1	B	917	ASP
1	B	1089	LEU
1	B	1114	MET
1	B	1141	LYS
1	B	1153	VAL
1	B	1173	LEU
1	B	1207	CYS
1	B	1229	THR
1	B	1231	TYR
1	B	1233	ASP
1	B	1255	LEU
1	B	1276	LEU
1	B	1329	LEU
1	B	1457	ILE
1	B	1473	GLU
1	B	1480	GLU
1	B	1705	ASN
1	B	1784	LEU
1	B	1805	TYR
1	B	1806	ASN
1	B	1838	THR
1	B	1869	ASN
1	B	1941	VAL
1	B	1961	MET
1	B	2044	LEU
1	B	2056	LEU
1	B	2088	VAL
1	B	2090	VAL
1	B	2095	LEU
1	B	2101	LYS
1	B	2166	LEU
1	B	2172	GLN
1	B	2175	PHE

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Mol	Chain	Res	Type
1	B	2178	MET
1	B	2203	ASP
1	B	2247	ASP
1	B	2295	PHE
1	B	2539	CYS
1	B	2545	LEU
1	B	2552	ARG
1	B	2564	ASN
1	B	2649	GLN
1	B	2664	LYS
1	B	2675	PHE
1	B	2677	LEU
1	B	2693	PHE
1	B	2722	SER
1	B	2723	MET
1	C	34	LEU
1	C	40	LEU
1	C	425	VAL
1	C	430	ASN
1	C	432	ILE
1	C	484	CYS
1	C	494	TRP
1	C	497	VAL
1	C	504	LYS
1	C	568	MET
1	C	653	LEU
1	C	662	VAL
1	C	663	LYS
1	C	685	THR
1	C	724	THR
1	C	731	PHE
1	C	749	VAL
1	C	750	ASN
1	C	767	ARG
1	C	773	LEU
1	C	777	LYS
1	C	798	ASN
1	C	807	GLU
1	C	818	THR
1	C	836	LEU
1	C	841	ILE
1	C	872	GLU

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Mol	Chain	Res	Type
1	C	881	LEU
1	C	916	CYS
1	C	1103	ARG
1	C	1109	LYS
1	C	1173	LEU
1	C	1202	LEU
1	C	1209	THR
1	C	1234	CYS
1	C	1256	TYR
1	C	1279	LEU
1	C	1339	LEU
1	C	1345	PHE
1	C	1373	GLN
1	C	1398	LEU
1	C	1415	PRO
1	C	1431	SER
1	C	1482	LEU
1	C	1490	ILE
1	C	1697	ARG
1	C	1799	MET
1	C	1821	TYR
1	C	1832	GLU
1	C	1838	THR
1	C	1846	MET
1	C	1922	LEU
1	C	1932	HIS
1	C	1939	LEU
1	C	1941	VAL
1	C	2062	ARG
1	C	2089	THR
1	C	2090	VAL
1	C	2095	LEU
1	C	2098	LEU
1	C	2102	MET
1	C	2166	LEU
1	C	2169	PHE
1	C	2203	ASP
1	C	2211	ILE
1	C	2215	LEU
1	C	2265	ARG
1	C	2269	THR
1	C	2291	VAL

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Mol	Chain	Res	Type
1	C	2528	CYS
1	C	2534	ARG
1	C	2539	CYS
1	C	2540	LEU
1	C	2564	ASN
1	C	2568	PHE
1	C	2692	SER
1	D	6	PHE
1	D	49	LYS
1	D	360	LEU
1	D	381	LEU
1	D	390	LEU
1	D	393	TRP
1	D	401	TYR
1	D	425	VAL
1	D	441	ASN
1	D	445	THR
1	D	467	GLU
1	D	504	LYS
1	D	512	LYS
1	D	525	MET
1	D	542	TYR
1	D	543	HIS
1	D	551	ILE
1	D	561	LEU
1	D	563	GLU
1	D	568	MET
1	D	569	ASN
1	D	572	CYS
1	D	650	GLN
1	D	651	TRP
1	D	677	TYR
1	D	700	ASP
1	D	705	LEU
1	D	717	GLN
1	D	762	THR
1	D	813	ARG
1	D	868	ILE
1	D	877	MET
1	D	878	GLN
1	D	895	LEU
1	D	911	PHE

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Mol	Chain	Res	Type
1	D	917	ASP
1	D	1089	LEU
1	D	1092	LEU
1	D	1098	LEU
1	D	1167	ASP
1	D	1173	LEU
1	D	1179	CYS
1	D	1187	GLU
1	D	1189	ILE
1	D	1211	CYS
1	D	1231	TYR
1	D	1242	THR
1	D	1244	ILE
1	D	1274	HIS
1	D	1319	LEU
1	D	1329	LEU
1	D	1339	LEU
1	D	1342	MET
1	D	1345	PHE
1	D	1381	ASP
1	D	1490	ILE
1	D	1829	ASN
1	D	1846	MET
1	D	1932	HIS
1	D	1941	VAL
1	D	1943	SER
1	D	2042	VAL
1	D	2089	THR
1	D	2092	ARG
1	D	2102	MET
1	D	2175	PHE
1	D	2232	LEU
1	D	2240	LEU
1	D	2247	ASP
1	D	2538	LEU
1	D	2539	CYS
1	D	2545	LEU
1	D	2558	LEU
1	D	2675	PHE
1	D	2684	GLU
1	D	2693	PHE
1	D	2731	TYR

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Mol	Chain	Res	Type
1	D	2733	TRP
1	D	2746	PHE
1	D	2777	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	GLN
1	A	421	ASN
1	A	469	GLN
1	A	543	HIS
1	A	782	ASN
1	A	783	ASN
1	A	816	ASN
1	A	914	HIS
1	A	1263	ASN
1	A	1794	GLN
1	A	1952	GLN
1	A	1962	ASN
1	A	2038	ASN
1	A	2182	HIS
1	A	2262	HIS
1	A	2553	HIS
1	A	2680	ASN
1	B	9	HIS
1	B	75	GLN
1	B	361	GLN
1	B	410	HIS
1	B	411	HIS
1	B	501	GLN
1	B	513	ASN
1	B	539	ASN
1	B	575	GLN
1	B	650	GLN
1	B	732	GLN
1	B	878	GLN
1	B	924	HIS
1	B	1176	ASN
1	B	1281	GLN
1	B	1362	HIS
1	B	1368	GLN
1	B	1451	ASN

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Mol	Chain	Res	Type
1	B	1508	GLN
1	B	1705	ASN
1	B	1963	GLN
1	B	2060	ASN
1	B	2253	GLN
1	B	2527	ASN
1	B	2587	GLN
1	B	2629	GLN
1	B	2630	ASN
1	B	2680	ASN
1	C	392	GLN
1	C	430	ASN
1	C	441	ASN
1	C	469	GLN
1	C	501	GLN
1	C	513	ASN
1	C	664	ASN
1	C	782	ASN
1	C	849	HIS
1	C	874	GLN
1	C	1176	ASN
1	C	1373	GLN
1	C	1385	HIS
1	C	1822	GLN
1	C	1826	ASN
1	C	1828	GLN
1	C	2093	ASN
1	C	2253	GLN
1	C	2551	ASN
1	C	2564	ASN
1	C	2614	GLN
1	D	41	ASN
1	D	411	HIS
1	D	794	GLN
1	D	1084	ASN
1	D	1137	GLN
1	D	1281	GLN
1	D	1290	HIS
1	D	1374	GLN
1	D	1508	GLN
1	D	1794	GLN
1	D	1852	GLN

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Mol	Chain	Res	Type
1	D	1919	ASN
1	D	2301	GLN
1	D	2551	ASN
1	D	2564	ASN
1	D	2566	HIS
1	D	2587	GLN
1	D	2629	GLN
1	D	2641	HIS
1	D	2680	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

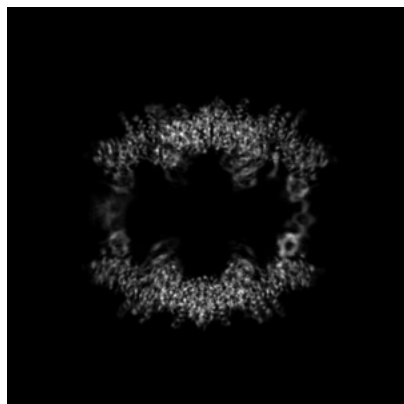
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28646. These allow visual inspection of the internal detail of the map and identification of artifacts.

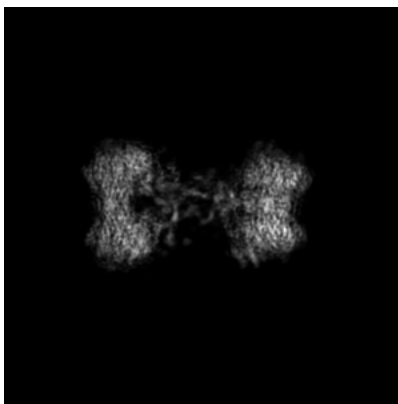
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

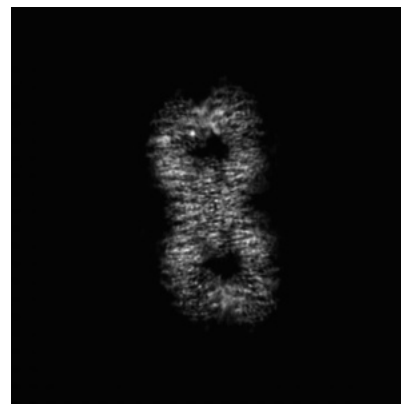
6.1.1 Primary map



X

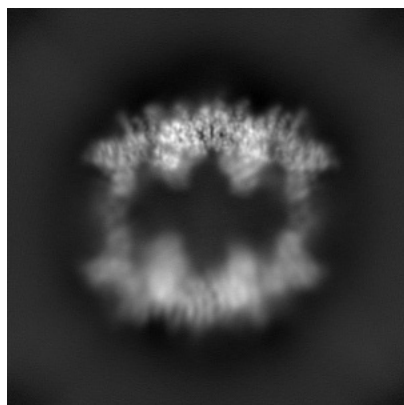


Y

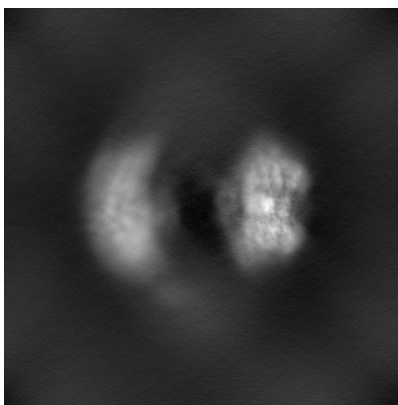


Z

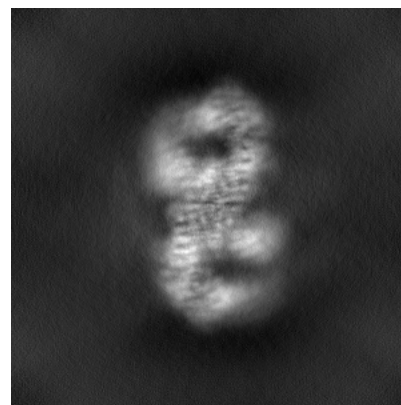
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

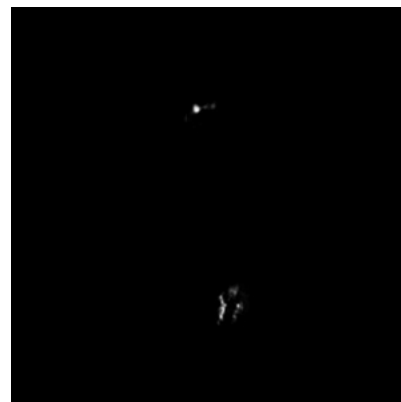
6.2.1 Primary map



X Index: 220

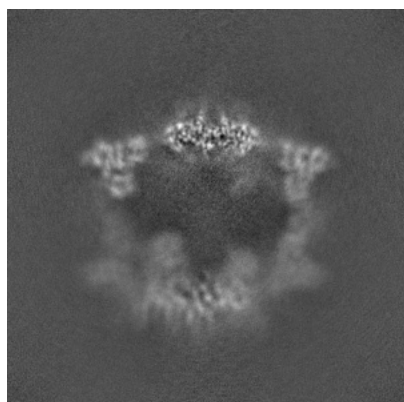


Y Index: 220

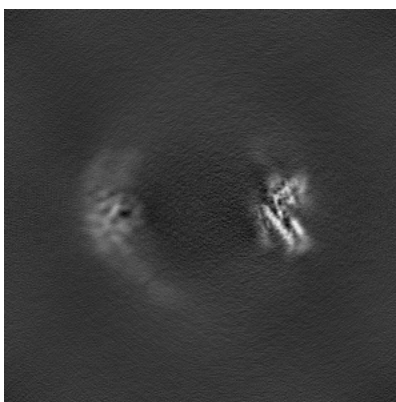


Z Index: 220

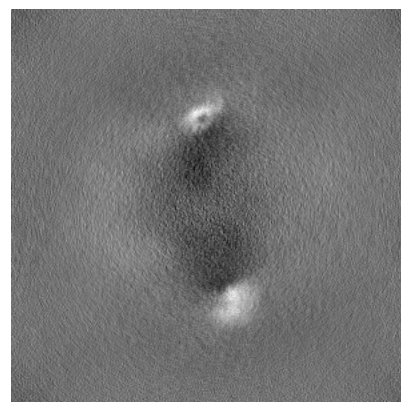
6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 195

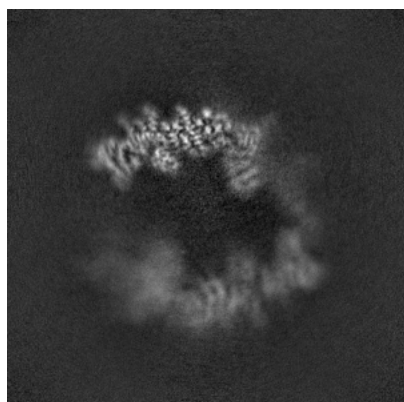


Y Index: 257

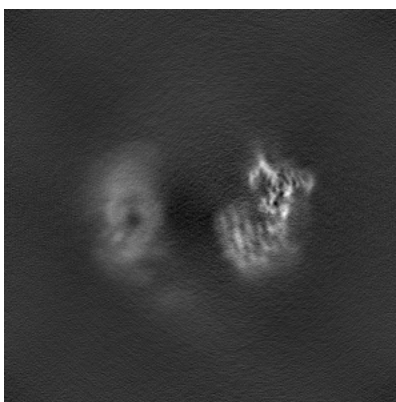


Z Index: 297

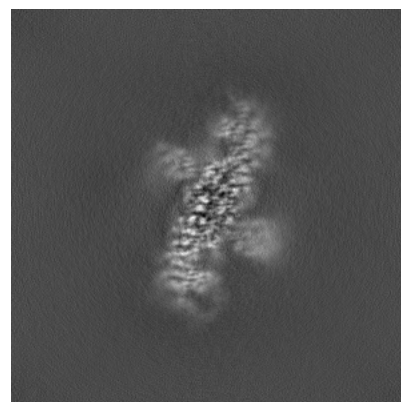
6.3.2 Raw map



X Index: 196



Y Index: 262

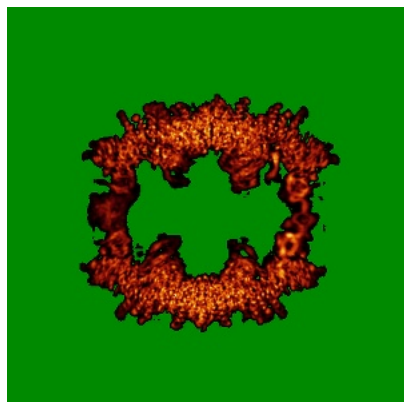


Z Index: 297

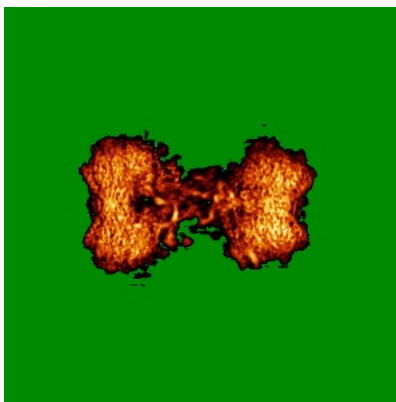
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

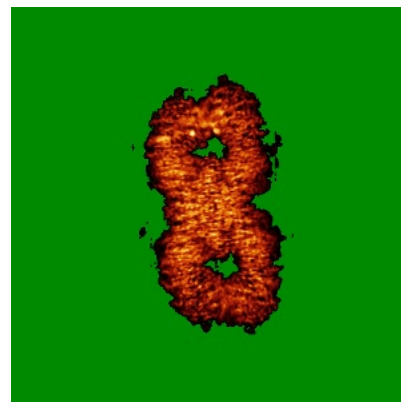
6.4.1 Primary map



X

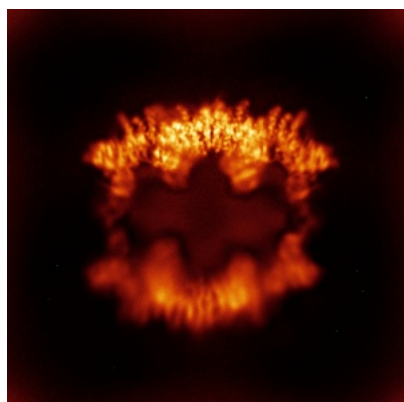


Y

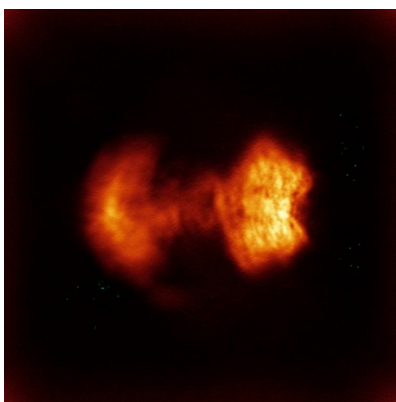


Z

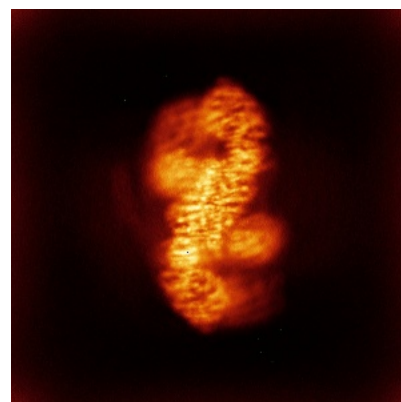
6.4.2 Raw map



X



Y

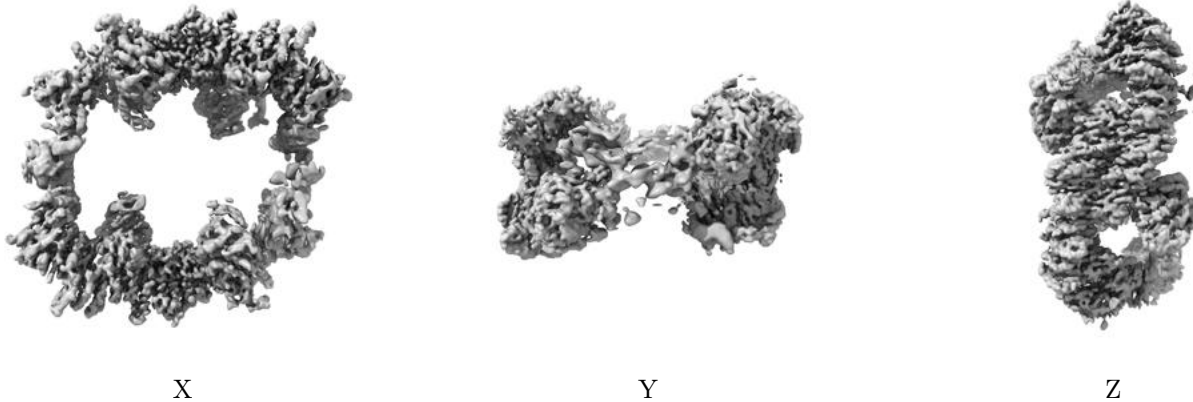


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

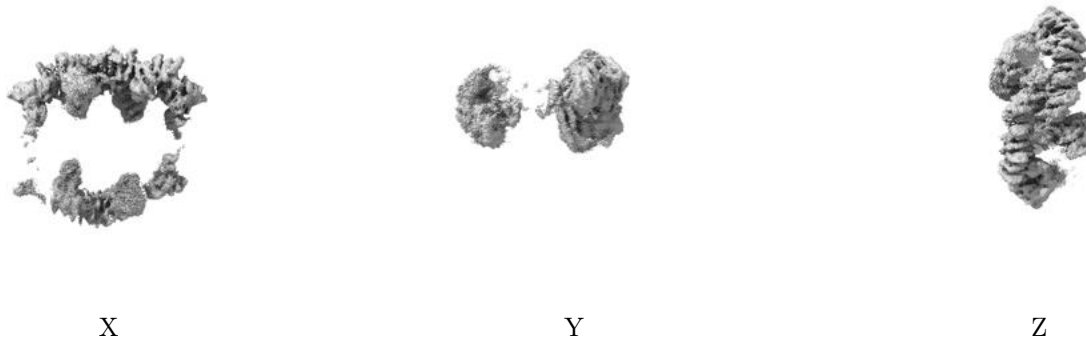
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

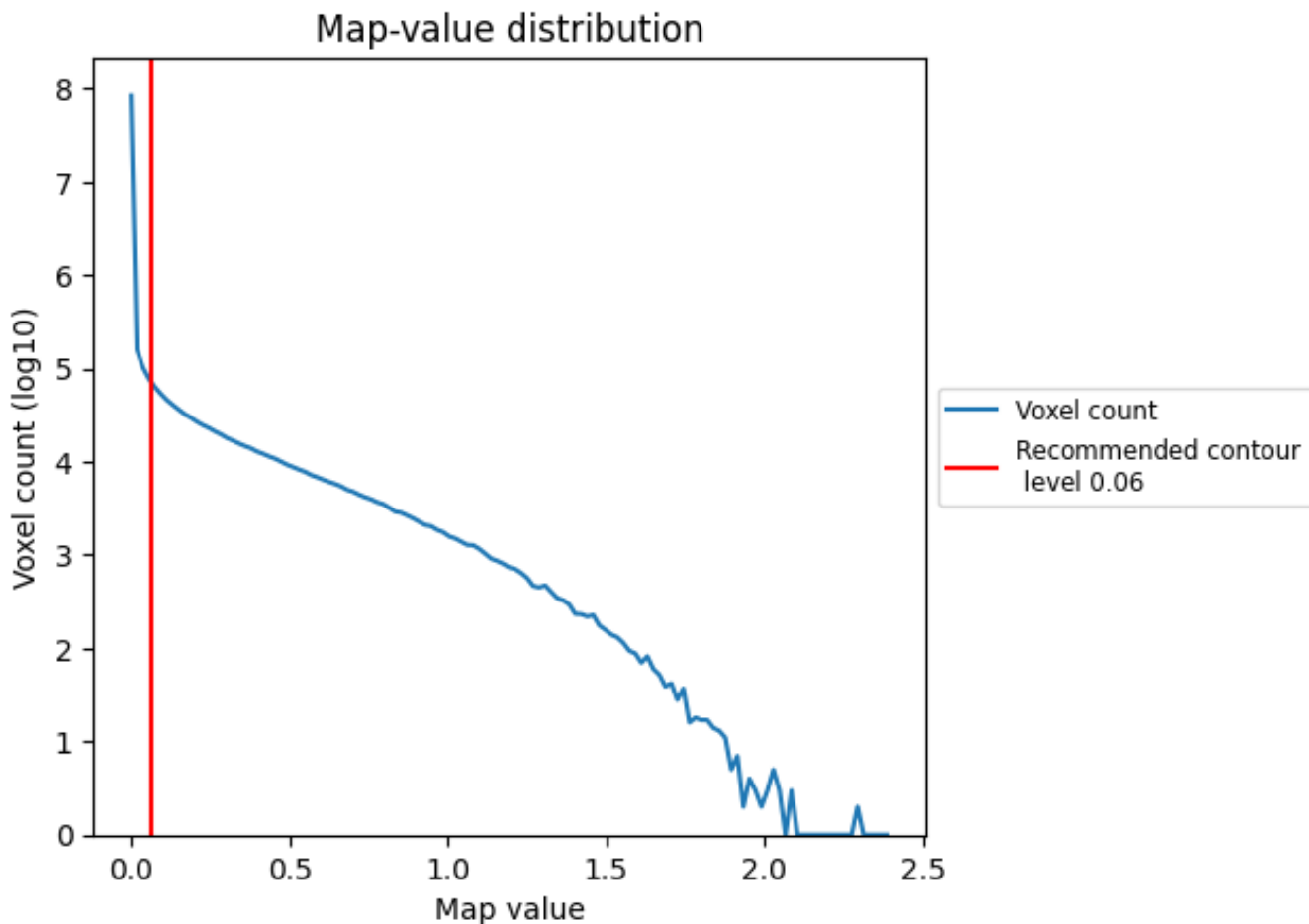
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

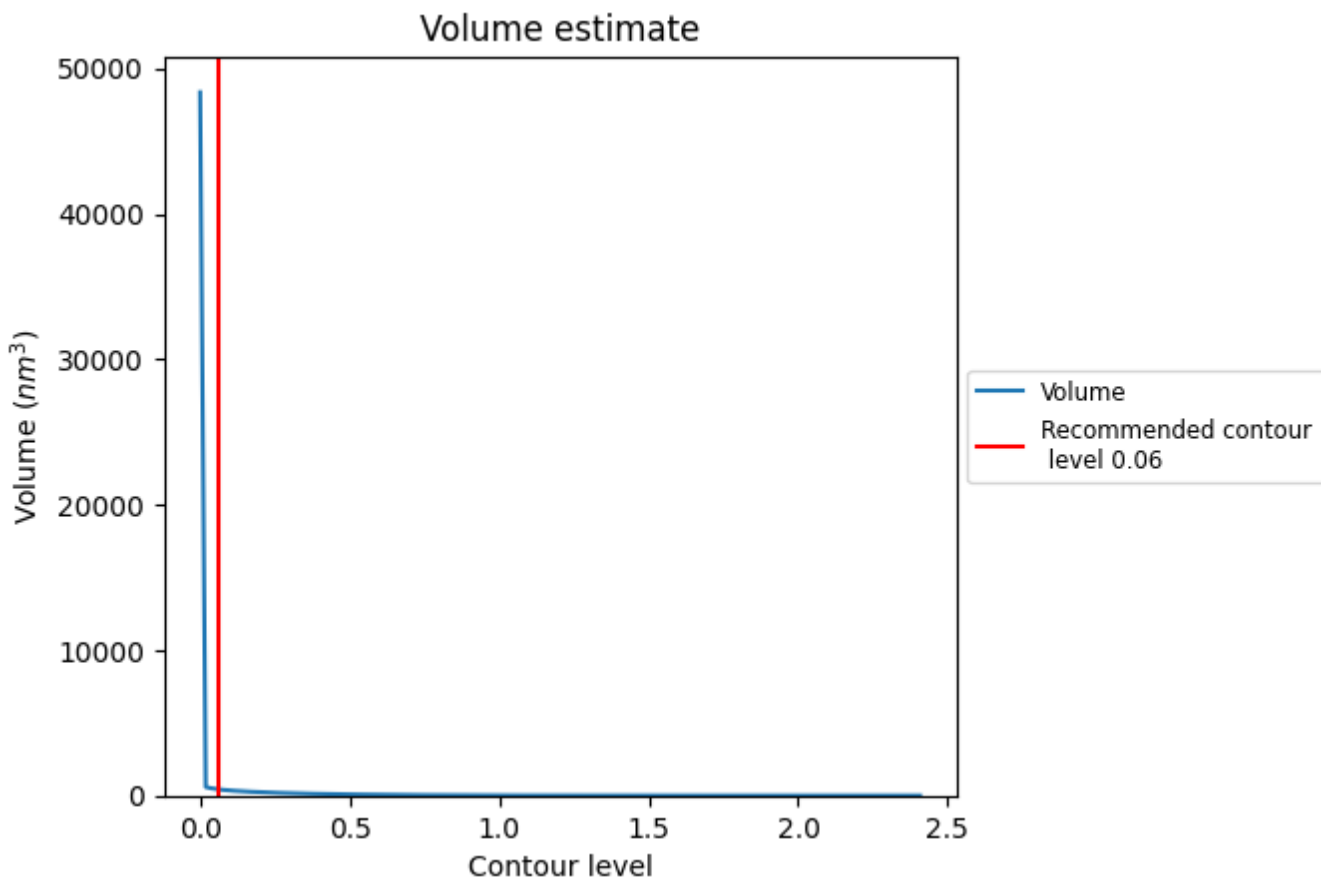
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

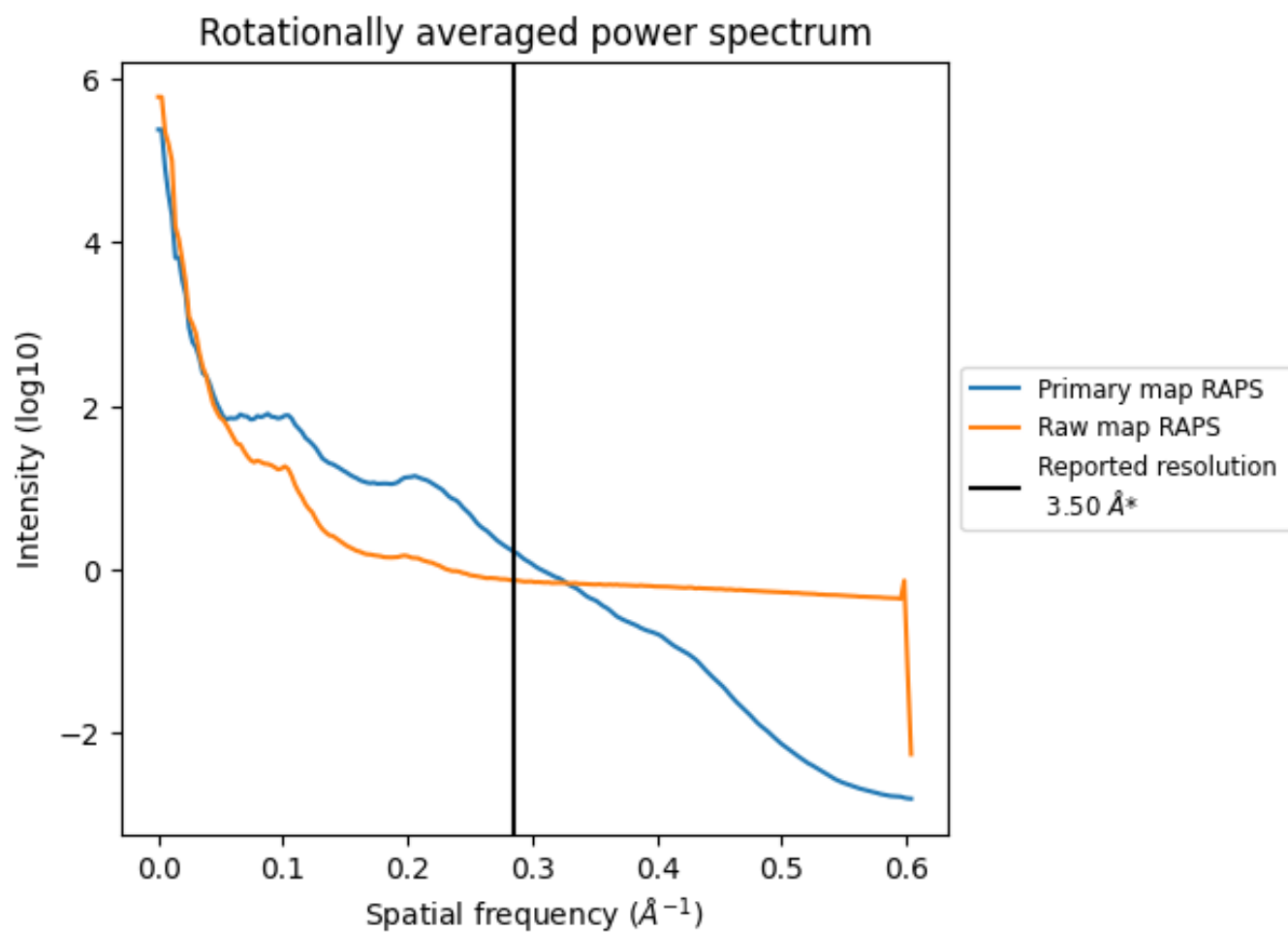
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm³; this corresponds to an approximate mass of 388 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

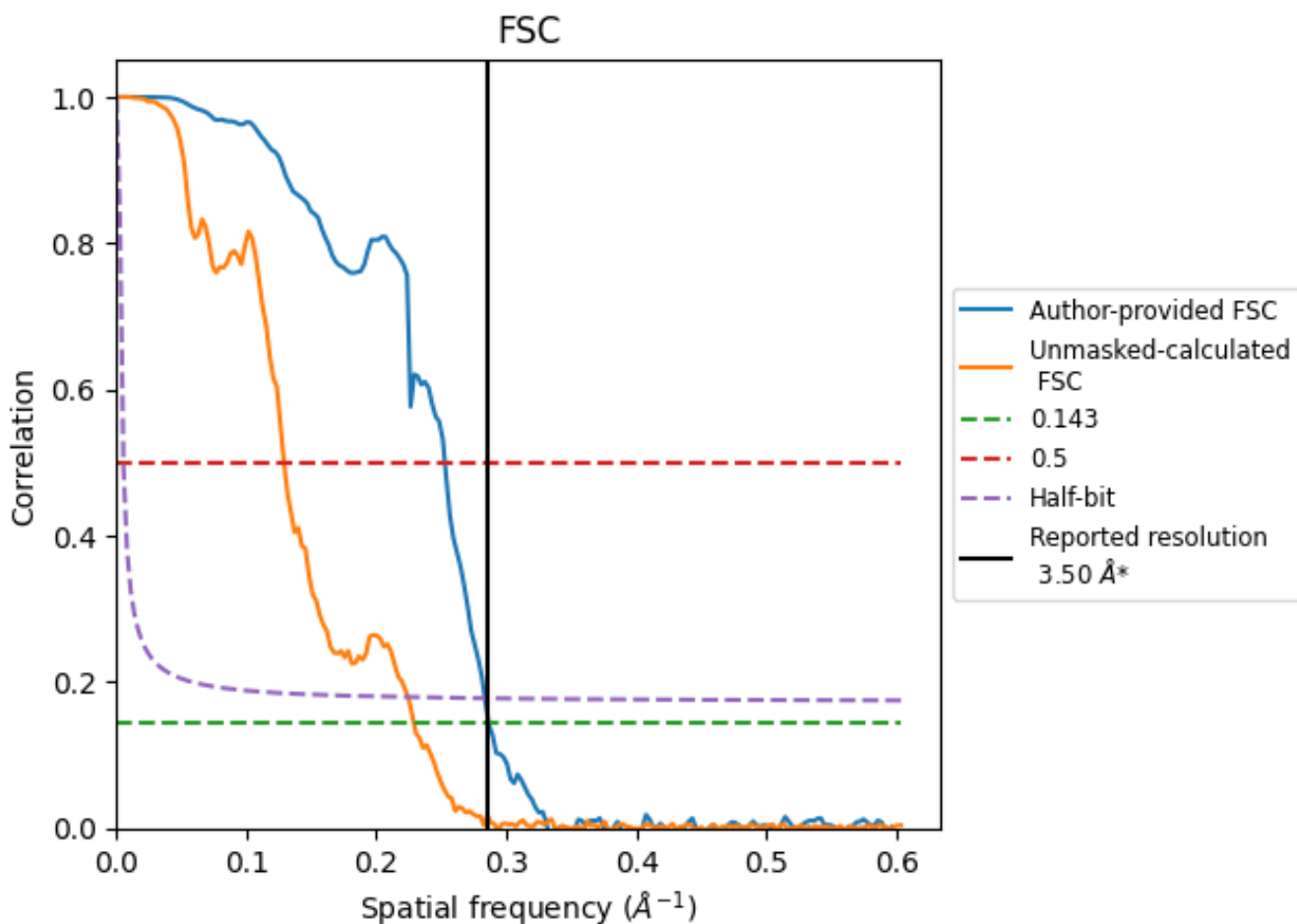


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

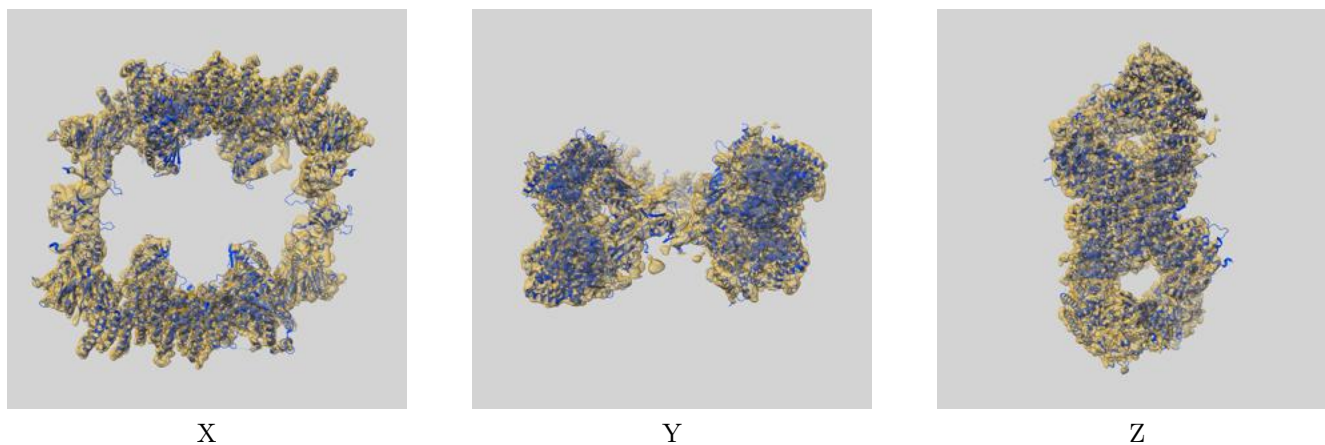
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.96	3.53
Unmasked-calculated*	4.37	7.75	4.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

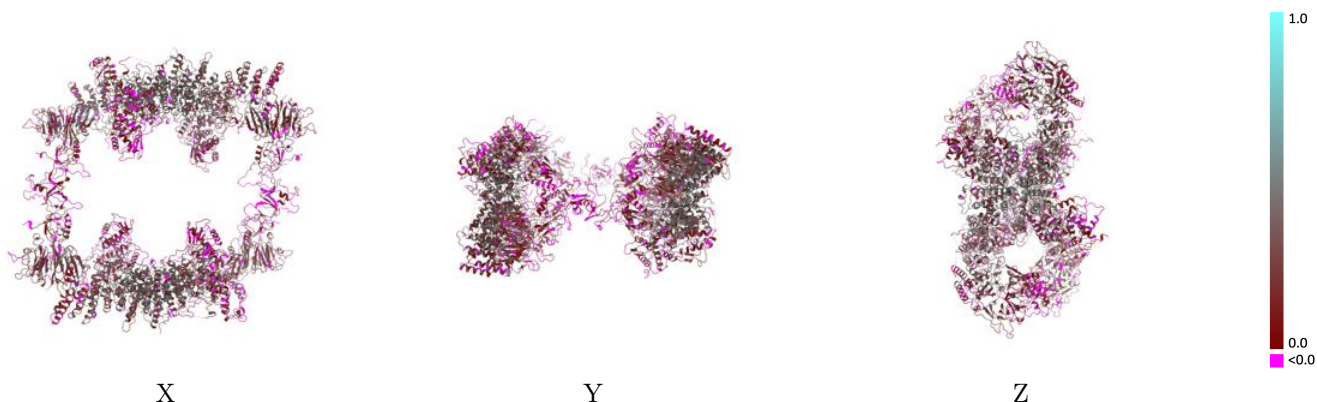
This section contains information regarding the fit between EMDB map EMD-28646 and PDB model 8EWI. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



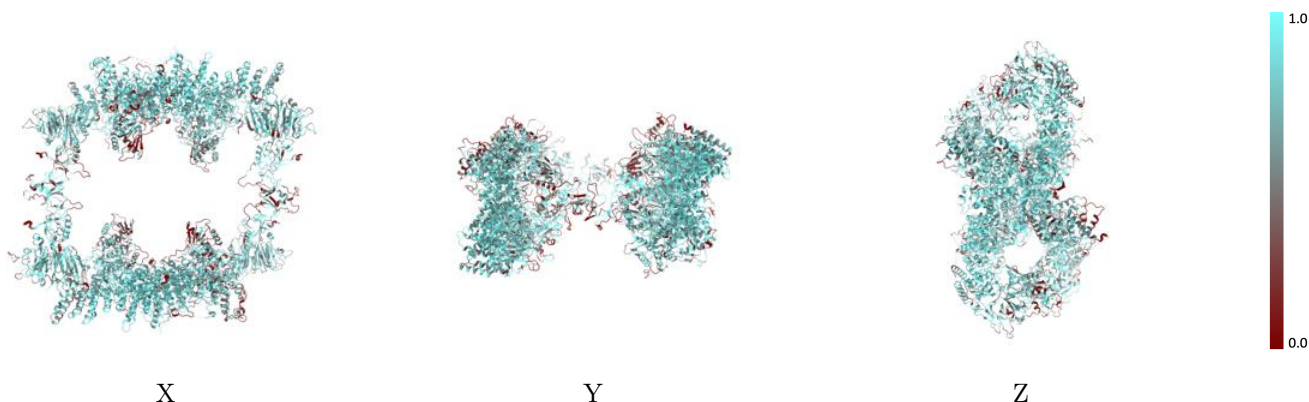
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



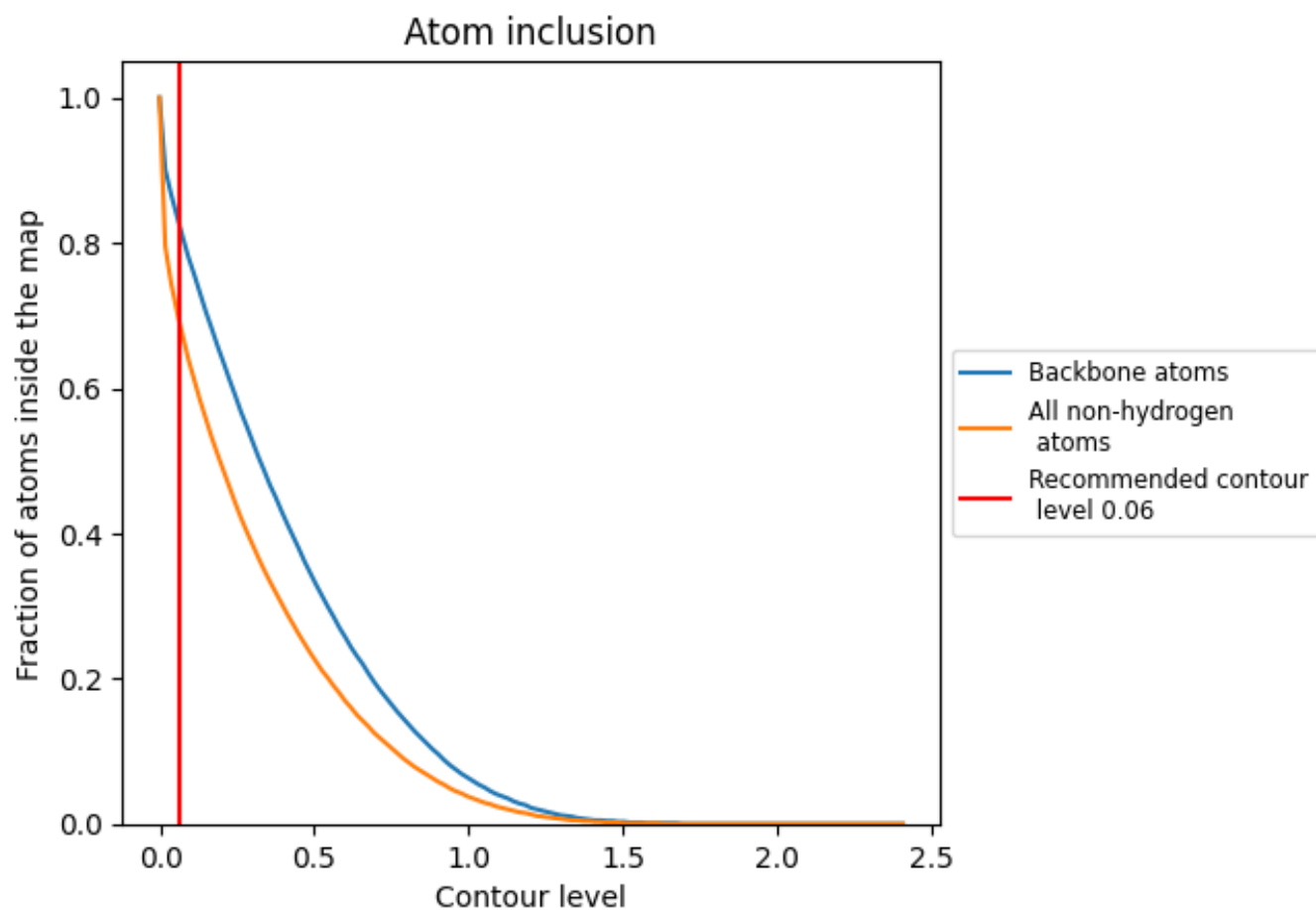
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).



9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6960	 0.2480
A	 0.7200	 0.2670
B	 0.6930	 0.2540
C	 0.6820	 0.2390
D	 0.6870	 0.2330

